वार्षिक प्रतिवेदन

ANNUAL REPORT

NATIONAL CHEMICAL LABORATORY

राष्ट्रीय रासायनिक प्रयोगशाला

2003-2004

वार्षिक प्रतिवेदन

ANNUAL REPORT
2003-2004

राष्ट्रीय रासायनिक प्रयोगशाला

NATIONAL CHEMICAL LABORATORY, PUNE

(Council of Scientific and Industrial Research, New Delhi)

Published by :
Dr. S. Sivaram
Director, NCL

Compiled & Edited by :
Publication & Science Communication Unit, NCL

Concept Design & Production by :
Rishi Jain - Idea Manufacturing Company, Pune.

CONTENTS

निदेशक की कलम से

राष्ट्रीय रासायनिक प्रयोगशाला का वर्ष 2003-2004 का वार्षिक प्रतिवेदन प्रस्तुत करते हुए मुझे प्रसन्नता हो रही है ।

समीक्षाधीन वर्ष के दौरान राष्ट्रीय रासायनिक प्रयोगशाला (एन.सी.एल.) ने अनेक क्षेत्रों में प्रगति का सिलसिला जारी रखा । हमने अपने भविष्य की रूपरेखा, लक्ष्य, मार्गदर्शी सिद्धान्त और नैतिक मूल्य तय किए । हमने अपने साझेदारों के हितों को ध्यान में रखा और हमारे वे साझेदार चाहे औद्योगिक ग्राहक हों, समाज हो, राष्ट्र हो, वैज्ञानिक समुदाय हो या फिर हमारे कर्मचारी हों, हमने उनकी अपेक्षाओं को परिभाषित किया । इससे एन.सी.एल. के प्रत्येक कर्मचारी को अपने साझेदारों की अपेक्षाओं के अनुरूप कार्य करने और संगठन के अन्दर अपनी भूमिका को स्पष्ट करने में मदद मिली है ।

पिछले वर्ष के दौरान प्रयोगशाला के प्रबन्धन/प्रशासन और कार्यों को सुव्यवस्थित करने के लिए अनेक संगठनात्मक परिवर्तन किए गए हैं । प्रयोगशाला के कार्यकलापों को अनेक ज्ञानाधारित क्षमताओं एवं संसाधन केन्द्रों में विभाजित किया गया है । प्रयोगशाला प्रबन्धन के सभी क्षेत्रों में सूचना प्रौद्योगिकी के नए उपक्रमणों की रूपरेखा बनाने और उन्हें कार्यान्वित करने के लिए सूचना प्रौद्योगिकी नीति सम्बन्धी एक दूरगामी दस्तावेज तैयार किया गया है । यह हमारा दृढ़ विश्वास है कि एक सक्षम, उपयुक्त एवं समकालीन विश्वस्तरीय सूचना प्रौद्योगिकी अवसंरचना के बिना राष्ट्रीय रासायनिक प्रयोगशाला विश्वस्पर्धी अनुसंधान एवं विकास संगठन नहीं बन सकता है ।

राष्ट्रीय रासायनिक प्रयोगशाला ने प्रौद्योगिकी विकास हेतु सरकारी धन की मदद से निजी उद्योगों की भागीदारी में अनेक बड़ी परियोजनाएँ प्रारंभ की हैं । इनमें से अनेक परियोजनाएँ अत्यन्त आन्तर्विद्यात्मक स्वरूप की हैं जिन पर एक साथ एक दल के रूप में कार्य करने के लिए एन.सी.एल. के अन्दर से ही ज्ञान की बहुविधाओं की विशेषज्ञता की आवश्यकता होगी । इनमें से अधिकांश परियोजनाओं से सम्बन्धित कार्यों में महत्त्वपूर्ण प्रगति हुई है । मुझे विश्वास है कि ऐसी विशाल विज्ञान एवं प्रौद्योगिकी परियोजनाएँ प्रौद्योगिकी सम्बन्धी एवं सामाजिक दोनों प्रकार की आवश्यकताएँ पूरी करने में एन.सी.एल. के सामूहिक सामर्थ्य का भरपूर उपयोग करेंगी ।

एन.सी.एल. ने मौलिक विज्ञान एवं प्रौद्योगिकी इन दोनों क्षेत्रों में अच्छा निष्पादन किया है । विश्व में उच्च गुणवत्ता वाले वैज्ञानिक साहित्य के सृजन में एन.सी.एल. भारत की ओर से प्रमुख योगदान देने वाली संस्थाओं में से एक है ।। अमरीकी केमिकल सोसायटी के दो प्रकाशनों (लैंगम्युर, नवम्बर 25, 2003 एवं जर्नल ऑफ ऑर्गेनिक केमिस्ट्री, नवम्बर 28, 2003) के मुखपृष्ठ पर अंकित एन.सी.एल. के वैज्ञानिक योगदानों को देखकर हमें प्रसन्नता हुई थी । वर्ष के दौरान उद्योगों को अनेक प्रक्रियाएँ प्रदर्शित की गईं । भारत के अन्दर और बाहर एन.सी.एल. के औद्योगिक ग्राहकों की एक अच्छी संख्या बनी रही । तेईस ग्राहकों को ठेके पर अनुसंधान सेवाएँ उपलब्ध कराई गईं, साठ ग्राहकों को तकनीकी सेवाएँ प्रदान की गईं और बयालीस ग्राहकों को परामर्शी सेवाएँ दी गईं । वर्ष 2003 में एन.सी.एल. ने भारत में इक्यावन पेटेण्ट और भारत के बाहर एक सौ अठारह पेटेण्ट फाइल किए ।

सहायता प्रदान करने वाले विभिन्न अनुभागों ने प्रयोगशाला के अनुसंधान और विकास सम्बन्धी कार्यकलापों को अपनी श्रेष्ठतम सेवाएँ प्रदान कीं । एन.सी.एल. ने अपने डिज़िटल संसाधनों (डिज़िटल सूचना संसाधन केन्द्र) की सुव्यवस्था के लिए एक नई इमारत का निर्माण किया । अस्सी के दशक के बाद एन.सी.एल. परिसर में निर्मित होने वाली यह पहली नई इमारत है । ज्ञानात्मक संगठन बनने की अपनी अभिलाषा के चलते एन.सी.एल. ने अपने कर्मचारियों की क्षमता और अनुभव को समुन्नत/समृद्ध करने के लिए प्रशिक्षण, व्याख्यान एवं संगोष्ठी जैसे अनेक कार्यक्रम आयोजित किए ।

आपके समक्ष प्रस्तुत वार्षिक प्रतिवेदन में वर्ष 2003-04 के दौरान प्रयोगशाला द्वारा सम्पादित विभिन्न कार्यकलापों की एक झलक देने का प्रयास किया गया है । प्रत्येक कार्यकलाप के मूल में रह कर उन पर कार्य करना हमारा अनवरत प्रयास रहा है और यही ही '' टीम एन.सी.एल.'' का अदम्य मनोभाव है । आशा है, आपको एन.सी.एल. का वार्षिक प्रतिवेदन पढ़ने में आनन्द प्राप्त होगा ।

मैं अपने सभी स्टाफ-सदस्यों, इस प्रयोगशाला की अनुसंधान परिषद और प्रबन्ध परिषद के सदस्यों तथा हमारे सम्माननीय साझेदारों द्वारा दिए गए समर्थन और सहयोग के लिए अपनी हार्दिक कृतज्ञता व्यक्त करता हूँ । उनका सहयोग एवं परामर्श अमूल्य रहा है ।

एस. शिवराम

(एस. शिवराम)

From The Director's Desk

I am pleased to present the Annual Report of the National Chemical Laboratory for the year 2003-04.

National Chemical Laboratory (NCL) continued to make major strides in several areas during the year under review. We defined our vision, mission as well as guiding principles and values. We mapped our stakeholders and defined the expectations of our stakeholders, may it be the industrial customers, society, the nation, the scientific community at large or our employees. This helped every employee of NCL to align his/her activities with the stakeholder expectations and clarify our respective roles within the organization.

During the past year several organizational changes have been made to facilitate the management of the laboratory and its functions. The activities of the laboratory have been grouped in terms of several Knowledge Competencies as well as Resource Centers. An IT vision document has been created to plan and implement new IT initiatives in all aspects of laboratory management. It is our firm belief that without an enabling world class IT infrastructure which is both appropriate and contemporary NCL can not be a globally competitive R&D organization.

NCL has embarked on several large projects by leveraging public funds for technology development in partnership with private industries. Many of these projects are highly inter-disciplinary in nature, requiring expertise drawn from multiple disciplines within NCL to work together as a team. Significant progress has been made on many of these projects. I believe that such large S&T projects can harness the collective strength of NCL in fulfilling both technology and societal needs.

NCL performed well in both basic science and technology. NCL is one of the leading contributors from India to high quality scientific literature in this world. We were pleased to see the scientific contributions from NCL highlighted on the cover page of two ACS publications (Langmuir, November 25, 2003 and J. Org. Chem., November 28, 2003). Several processes were demonstrated to industries during the year. NCL continued to have an impressive list of industrial customers, both within and outside India. Contract research services were provided to twenty-three customers, technical services to sixty customers and consultancy services to forty-two customers. The year 2003 saw NCL filing fifty-one patents in India and one hundred and eighteen patents outside India.

The various support services rendered excellent support to the R&D activities of the laboratory. NCL added a new building to house its digital resources (Digital Information Resource Center), the first new building to come on campus since the early eighties. In its aspiration to become a 'learning organization' NCL organized several programmes to enrich its human resources in terms of training, lectures and seminars.

The Annual report that you are now holding in your hands attempts to capture the flavour of various activities that the laboratory undertook during the year 2003-04. Underlying each and every activity has been the incessant quest for excellence and the indomitable spirit of 'Team NCL'. I hope you enjoy reading the Annual Report of NCL.

I wish to gratefully acknowledge the support and cooperation of all my staff, CSIR, members of the Research and Management Councils of this laboratory and our valued stakeholders. Their assistance and advice has been invaluable.

S. Sivaram

(S. Sivaram)

VISION

- To be a globally recognized and respected R&D organization in the area of chemical sciences and engineering
- To become an organization that will contribute significantly towards assisting the Indian chemical and related industries in transforming themselves into globally competitive organizations
- To become an organization that will generate opportunities for wealth creation for the nation and, thereby, enhance the quality of life for its people

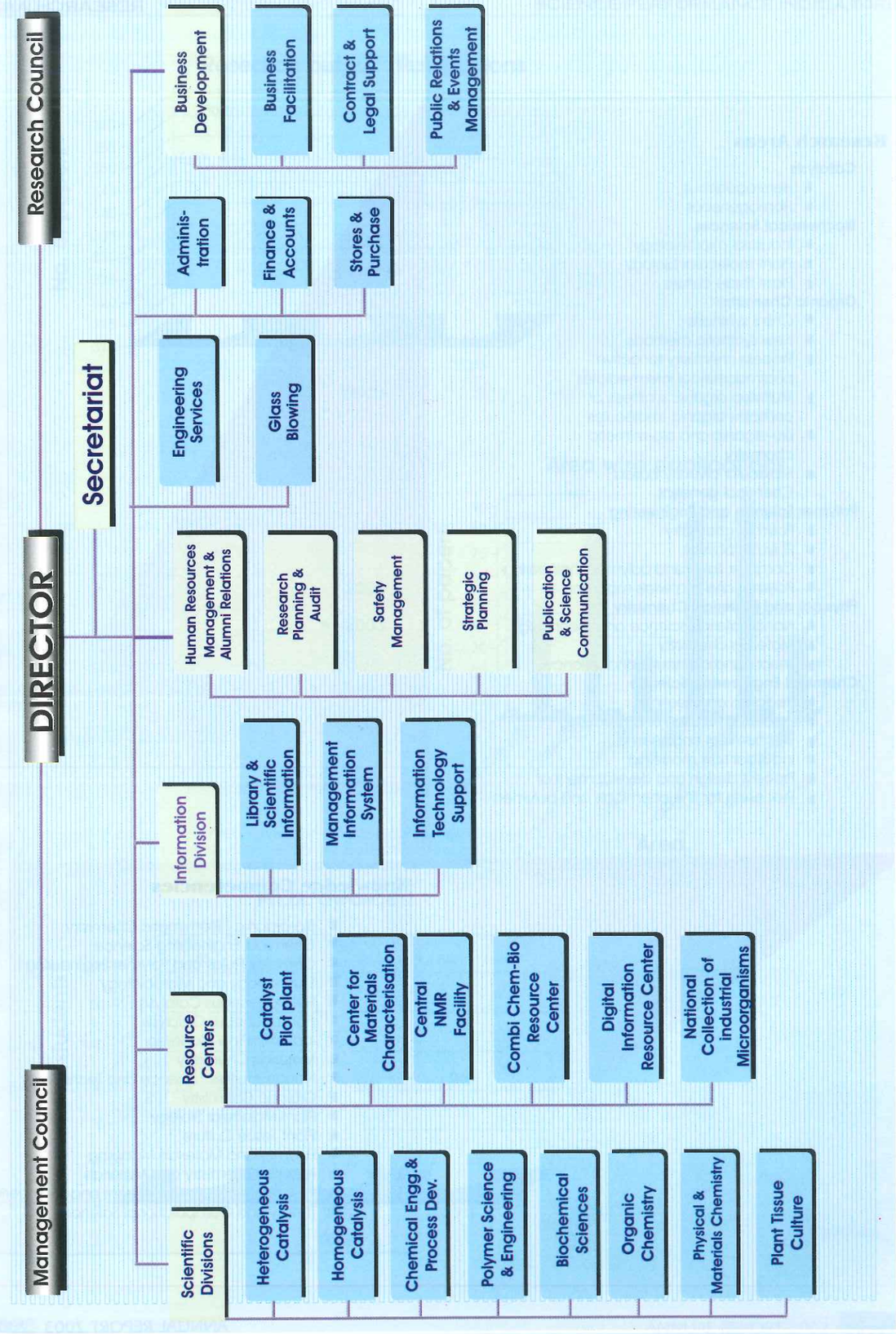
MISSION

- To carry out R&D in chemical and related sciences with a view to eventually deliver a product, process, intellectual property, tacit knowledge or service that can create wealth and provide other benefits to NCL's stakeholders
- To build and maintain a balance portfolio of scientific activities as well as R&D programmes to enable NCL to fulfill the demands of its stakeholders, present and future
- To create and sustain specialized Knowledge Competencies and Resource Centers within NCL which can provide support to all stakeholders of NCL

GUIDING PRINCIPLES & VALUES

- To be deeply committed to the success of our stakeholders
- To create and sustain a self driven and self managed learning organization with a high degree of internal and external transparency
- To encourage a culture of collective and principle-centred leadership
- To value the dignity of the individual and deal with people with a sense of fairness and without bias, prejudice or favour
- To nurture the highest standards of integrity and ethical conduct

ORGANISATIONAL CHART



Research Areas

Catalysis
- Heterogeneous
- Homogeneous

Biochemical Sciences
- Industrial microbiology
- Plant molecular biology
- Plant tissue culture

Organic Chemistry
- Chiral synthesis
- New synthetic methods
- Process chemistry for active pharmaceutical intermediates
- Multistep organic synthesis of complex organic molecules
- Bio-organic and bio-mimetic chemistry
- Molecular diversity based Chemical genetics

Polymer Science and Engineering
- Polymer chemistry
- Polymer physics
- Complex fluids and polymer engineering
- Polymer and materials modeling

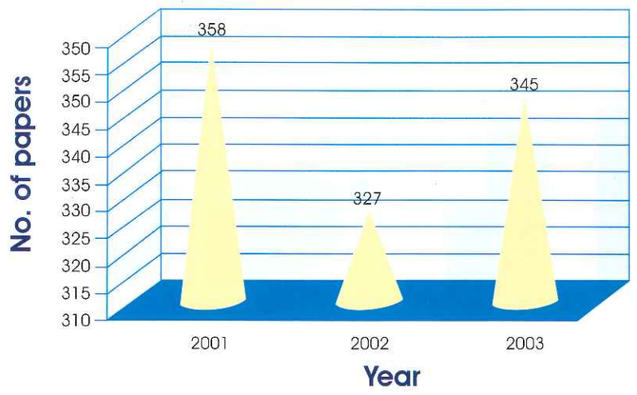
Physical and Materials Chemistry
- Nanomaterials science and technology
- Materials chemistry
- Theory and computational science

Chemical Engineering Science
- Reaction engineering
- Process simulation and modeling
- Biochemical engineering
- Industrial flow modeling
- Process design and development of
- Processes for fine chemicals and polymers

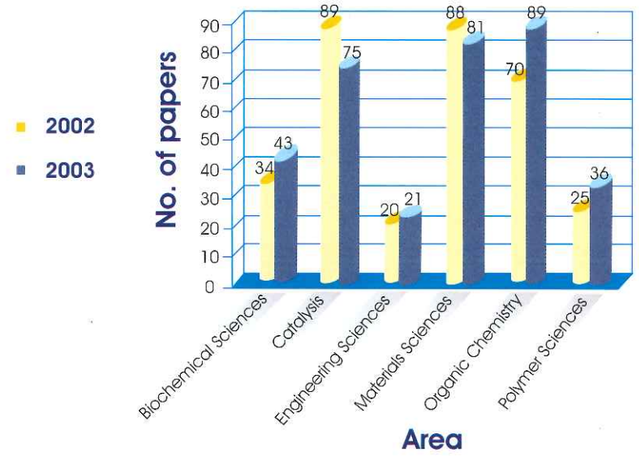
Knowledge Competencies

- Bio-organic / Biomimetic Chemistry
- Chemical Engineering Science
- Complex Fluids and Polymer Engineering
- Enzymology and Microbiology
- Heterogeneous Catalysis
- Homogeneous Catalysis
- Industrial Flow Modeling
- Materials Chemistry
- Nanomaterials : Science and Technology
- Organic Chemistry
- Plant Molecular Biology
- Plant Tissue Culture
- Polymer and Materials Modeling
- Polymer Chemistry and Materials
- Process Design, Development and Engineering
- Theory and Computational Science

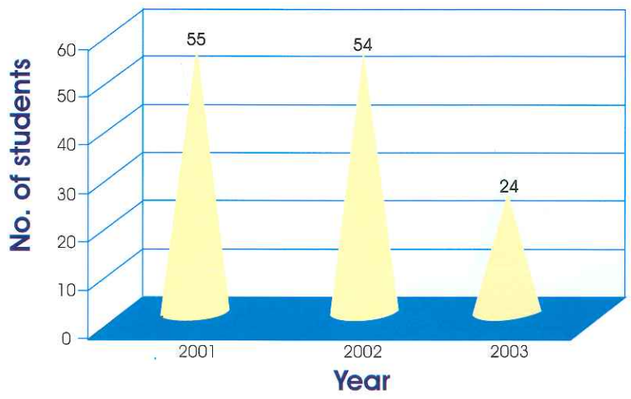
Research output : Publications



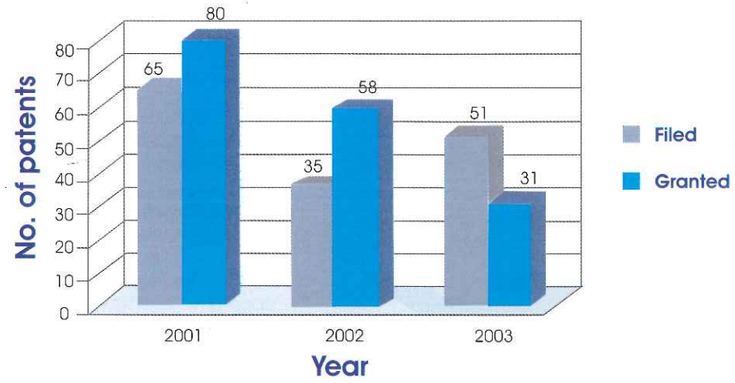
Area wise publications



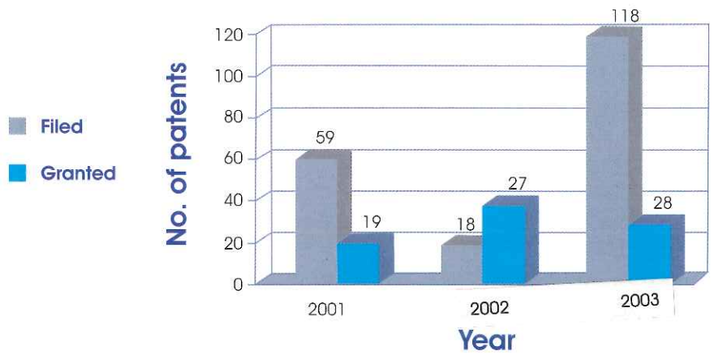
Ph.D. awarded



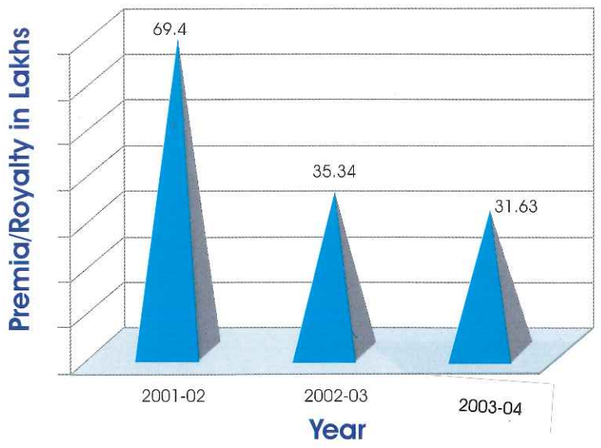
Indian patents : Filed and granted



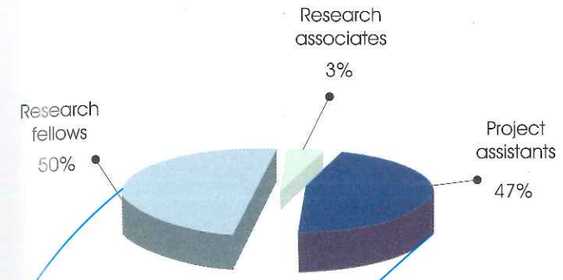
Foreign patents : Filed and granted



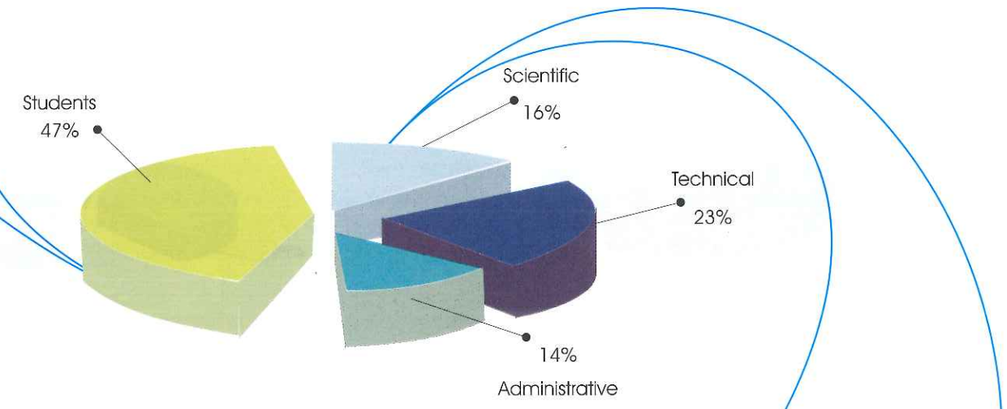
Premia/royalty earnings



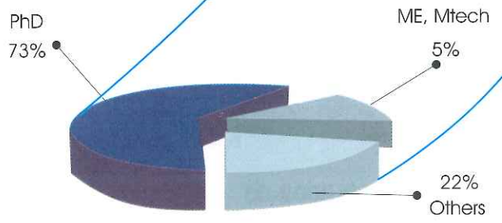
Research students & project assistants



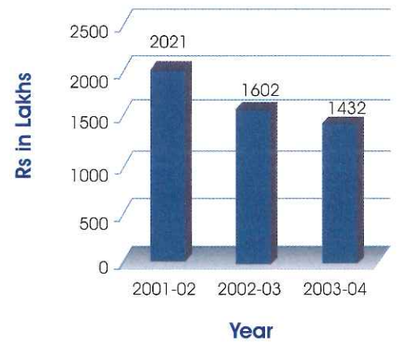
Total staff (1678)



Scientists : Qualification

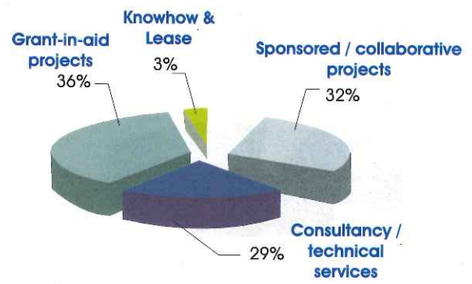


External Income



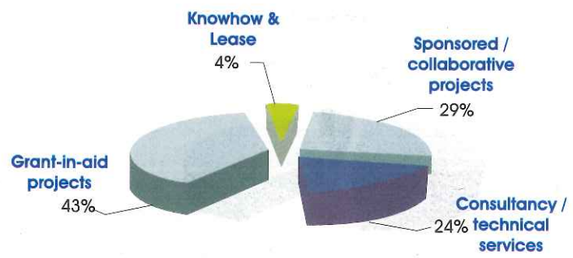
Project wise break-up of ECF : 2002-03 and 2003-04

Total Rs. 1602 Lakhs



2002-03

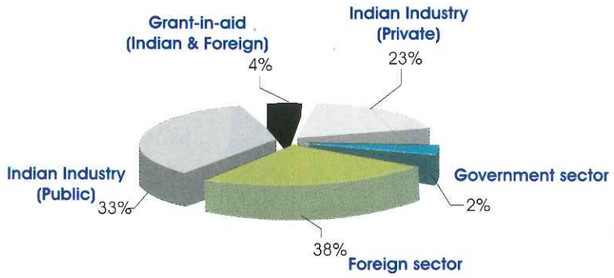
Total Rs. 1432 Lakhs



2003-04

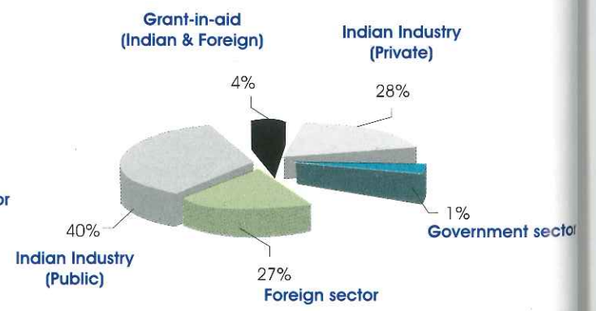
ECF by source : 2002-03 and 2003-04

Total Rs. 1602 Lakhs



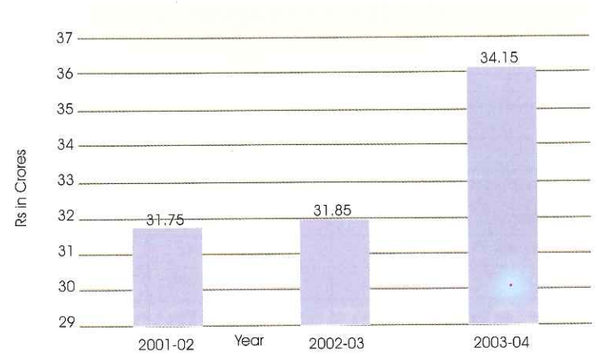
2002-03

Total Rs. 1432 Lakhs



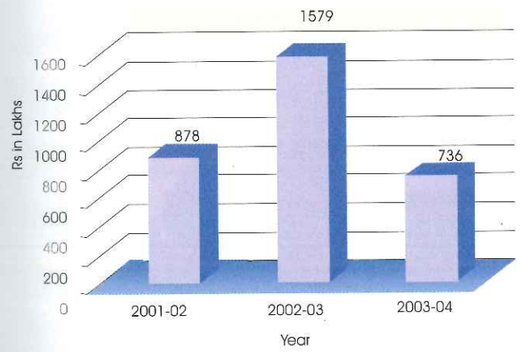
2003-04

CSIR Budget

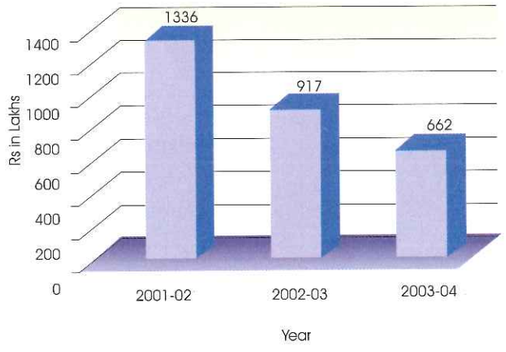


CSIR Budget :	31.75	30.00	30.07
Network Projects :	—	01.85	04.08

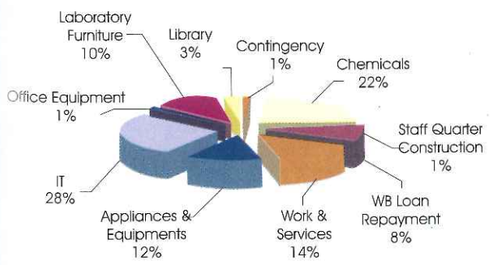
Laboratory reserve : LR expenditure



Laboratory reserve : Receipts

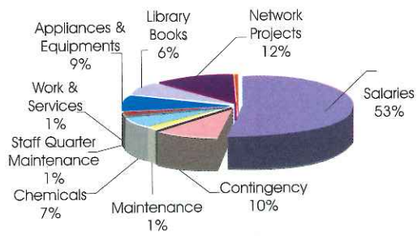


Expenditure : Laboratory reserve (Rs 736 Lakhs)



2003-04

Expenditure : CSIR and Network Projects (Rs 3415 Lakhs)



2003-04

CAPITAL AND RECURRING EXPENDITURE ON R&D (2002 – 2004)

Rs. in Lakhs

Source	Capital		Recurring	
	2002-03	2003-04	2002-03	2003-04
CSIR	288	313	267	251
Lab Reserves	1027	376	97	165
Projects *	236	856	170	478
Network Projects	26	342	2	212
Total	1577	1887	536	1106
%	75%	63%	25%	37%

* - excluding NMITLI projects

ONGOING PUBLICLY FUNDED MISSION MODE AND INTERNAL PROJECTS

Sr. No.	Description	Amount in Lakhs
1	CSIR NMITLI	411
2	DST	24
3	DBT	188
4	OTHERS *	115
5	X FIVE YEAR PLAN NETWORK PROJECTS	674
6	INTERNAL PROJECTS **	137
	Grand Total	1549

* - NPSM / SDC / McNIGHT etc.
** - Funded from Lab Reserve of NCL

SCIENTIFIC BUDGET (2003 - 04)

Funding Source

Rs. in Lakhs

	Recurring	Capital	Total
CSIR	226	212	438
LR	190	476	666
TOTAL	416	688	1104

RESEARCH & DEVELOPMENT REPORTS

ANNUAL REPORT 2003-2004

1. Biotechnology

1.1 Basic biochemical sciences

1.1.1 Enzymology

Purification and characterization of industrially important hydrolytic enzymes such as endoglucanases, xylanases, proteases, chitinases and pectate lyases have been carried out to elucidate their structure-function relationships. The purification and immobilisation of monoxygenases which are involved in biotransformation of pharmaceutically important compounds such as 19 HETE & 20 HETE is being carried out.

Microbial nucleases play an important role in replication, repair, recombination and restriction while extracellular enzymes have a role in nutrition. The extracellular nucleases with high activity from a thermophilic strain of *Streptomyces thermonitrificans* have been identified and their mode of action has been studied. Both the nuclease Stn α and β cleaved DNA endonucleolytically liberating 3'- and 5'-mononucleotides, respectively.

The equilibrium unfolding of Rnase Rs from *Rhizopus stolonifer* and the pH dependence to chemical and thermal denaturation have been investigated.

FemX, a non-ribosomal peptidyl transferase initiates synthesis of interchain peptide of peptidoglycan in bacterial cell wall, was found only in gram positive bacteria. Thus it makes it important pathogen-specific drug target. Getting the molecular structure solved would enable to reveal the basis of catalytic activity and will also help in designing the inhibitor that will have pathogen specific action keeping the natural flora intact. The protein was purified to homogeneity and further characterization is in progress.

1.1.2 Glycobiology

The lectin from *Artocarpus hirsuta,* which shows similar structure to Jacalin differs in the sugar binding specificity. It also shows a pH-dependent aggregation on thermal denaturation. A lectin from chickpea with unusual sugar specificity and another from drumstick with complex sugar specificity have been purified. Further studies on their properties are in progress.

A lectin from an endophytic fungus *Fusarium* sp. has been purified. This lectin is produced in the sporulation stage. The characterization of its properties is in progress.

1.1.3 Structural biology

Structural studies of lectins and protease inhibitors

Crystal structure analysis of galactose specific lectin from *Artocarpus hirsuta* at 2.5 Å resolution was completed. A lectin from chickpea (*Cicer arietinum*) with complex specificity has been crystallized and X-ray diffraction data were collected up to 2.3Å resolution. The structure of a galactose specific lectin from *Erithrina indica* has been determined at 3.5Å resolution using molecular replacement method. The structure was found closely related to *Erythrina corollodendron* lectin. A galactose specific lectin from *Trichosanthes dioica* was purified and crystallised. A cysteine protease inhibitor was purified from a tuber of *Dioscorea alata* and its crystallisation is in progress.

Studies on penicillin acylases and conjugated bile salt hydrolases

These studies aim at elucidating the structure and mechanism of enzyme activity and post-translational processing of penicillin V acylases (PVA) as well as the relationship between conjugated bile salt hydrolases (BSH) and PVA. The BSH protein was crystallized in two crystal forms. Data were collected at 2.4 Å from one crystal form and at a lesser resolution from the other. A Penicliin G Acylase (PGA) from *Kluyvera citrophila* has been purified and crystallized to study its post-translational processing and structure-activity relation.

Structural studies of c-phycocyanins from three cyanobacteria

Cyanobacteria and eukaryotic red algae possess large light-harvesting protein complexes called phycobilisomes, which effectively capture light energy and transfer it to the photosystem II. These complexes are located on the surface of the photosynthetic membranes. Phycobilisomes are composed of rods and a core which are highly organized by various phycobiliproteins and linker peptides. The light harvesting phycobiliprotein C-phycocyanin (C-PC) from three cyanobacterial species namely *Spirulina sp.* (from fresh water), *Phormidium sp.* (from marine water) and *Lyngbya sp.* (from marine water) have been crystallised and their structure was solved using X-ray diffraction data close to 3.0 Å resolution. The subunit of C-PC consists of two peptide chains α and β. This (α/β) heterodimer associates to form a ring shaped trimer. The stable functional unit is a hexamer of two stacked trimers.

Bioinformatics and database analysis

Accurate prediction of protein structure still remains a gray area of research in structural biology. Presently several well refined crystal structures are available in the protein data bank. An analysis of nearest neighbor interactions of residues will help in classifying local folds of the sequence. The neighbour residue interactions in selected protein structures have been analyzed.

A database on defective proteins causing genetic disorders in humans is in the preliminary stages of development. We plan to include in this database the analysis of lethal mutations and their effect on three-dimensional structure of functional proteins.

Structural studies of novel carbohydrate derivatives

Isonucleosides are a novel class of nucleosides in which nucleobases are linked to the non-anomeric carbons of carbohydrates. They are recognised as therapeutic agents with lesser toxicity and possessing higher selectivity towards viral and cancer cells. Half a dozen compounds, mainly with substitutions at C-2 position, have been analysed through X-ray crystallography for understanding their conformational changes and crystal packing.

1.1.4 Microbiology

Study of dimorphism in *Benjaminiella poitrasii*

Benjaminiella poitrasii, a dimorphic zygomycetous fungus possesses three glutamate dehydrogenases, one requiring NAD while the other two use NADP as a coenzyme. In the activity staining after electrophoresis on native polyacrylamide gel NAD- dependent glutamate dehydrogenase revealed the presence of one enzyme that was expressed in both, yeast- and mycelium-form cells. While in case of NADP- dependent glutamate dehydrogenase two distinct activity bands that were differentially expressed in yeast- and mycelium-form cells were seen. Interestingly, during yeast-mycelium transition and reverse, quantitative changes in form-specific native NADP-dependent glutamate dehydrogenase activities were seen. For the first time the significance of differential expression of these enzymes during morphological transition in *B. poitrasii* has been suggested.

The purification and characterization of 2 NADP- and one NAD-dependent glutamate dehydrogenases is in progress. The cloning NADP-glutamate dehydrogenase gene from *B.poitrasii* in *E.coli* has been carried out. The studies involving the expression of the gene at different morphological stages to understand the regulatory mechanisms at the molecular level is underway.

Studies on chitin metabolizing enzymes of *Metarhizium anisopliae*

The possible contribution of extracellular constitutively produced chitin deacetylase by *Metarhizium anisopliae* in the process of insect pathogenesis has been evaluated. Chitin deacetylase converts chitin, a β-1,4-linked *N*-acetylglucosamine polymer into its deacetylated form chitosan, a glucosamine polymer. It has been suggested that this enzyme may have a dual role in modifying the insect cuticular chitin for easy penetration as well as for altering its own cell walls for defense from insect.

Use of mycoharvester to harvest spores of insect-pathogenic fungi

1.2 Biotechnology

1.2.1 Microbial technology

1.2.1.1 Biotransformation

Arachidonic acid is an important essential fatty acid needed by the body. It is a long chain fatty acid with 20 carbon atoms and 4 double bonds. It serves as the main parent compound for the biosynthesis of many physiologically important compounds such as prostaglandin, leukotrienes, thromboxanes and vasoactive compounds like 19 HETE and 20 HETE. 20 HETE is a potent vasoconstrisctor and is present in most parts of our body including lungs, kidneys and brain. The concentration of this compound increases in cases of injury or damage to the tissues thus causing constriction of the blood vessels and thereby avoiding loss of blood. 19 HETE on the other hand is an antagonist of 20 HETE and serves its action by bringing about vasodialation. This fact is exploited and the production of this compound is aimed at, for future use as drug in hypertension and asthma. Chemical synthesis of these compounds is difficult because of the inactive carbon center which lies at the 20th position in arachidonic acid. Therefore, interest was diverted towards the use of yeasts like *Candida bombicola,* which posses the mono-oxygenase enzyme system to bring about the above reaction with great ease.

The fungus *Trichothecium* enantioselectively reduces acetophenons and its analogous to the corresponding (R)-alcohol. Work in other enantioselective oxidation-reduction reactions for other compounds is in progress.

Biotransformation of key pharmaceutical intermediates

Under this project four chiral compounds (phenyl ethyl maleimide, doxazosin mesylate, repaglinide and diethyl 3-hydroxy glutarate) which have commercial potential were identified. The objective is to develop a laboratory scale biocatalytic route for their production. Currently these compounds are produced by multi-step synthetic routes. Under this program four lipases have been tested for performing reactions for two (phenyl ethyl maleimide and doxazosin mesylate) of the above products and the initial results are encouraging.

Biotransformation of tea catechins to theaflavins using tea polyphenol oxidase

The objective is to design an immobilized enzyme bioreactor for continuous conversion of tea catechins to theaflavins. Black tea pigments, besides being the major components of black tea liquors which form part of daily dietary intake of tea drinking populations, can also be used as safe food and pharmaceutical colorants. Some of the isolated catechins and theaflavins (TF) have antioxidant, anti-microbial and anti-tumor activities. Normally, black CTC teas have 1-2% TF and 10-17% thearubigins (TR) in mixed form. It is possible to convert tea catechins specifically to TF through isolated enzymes. It may be possible to immobilize these enzymes and create a bioreactor

for the production of TF. This enzyme was immobilized onto the polymeric matrices developed at NCL so as to improve stability and reusability of polyphenol oxidase.

1.2.1.2 Textile

Development of cellulase from an extremophilic actinomycete for textile industry

Due to recent increase in environmental pressures in the textile industries, cellulases are expected to play a crucial role in developing an eco-friendly technology. The basis for the application of cellulases in biofinishing of denims is the action of cellulases, specifically endoglucanases on cellulose fibers. The traditional use of pumice stone in a water-loaded tumbling machine produces severe wear and loss of tensile strength of the fabric when used to achieve high degree of indigo fading. In addition, use of pumice stones causes clogging of outlet of the machine. Thus, introduction of cellulase enzymes to create the required effect without the use of stones and increasing their compatibility with other chemical processes is one of the thrust areas of research in textile industry.

A novel alkalothermophilic *Thermomonospora* producing alkali and thermostable cellulose has been identified. The cellulase was found to be highly effective with respect to i) reducing hairiness, ii) total weight loss, iii) impartation of softness, iv) washdown effect, v) back staining, vi) colour contrast and vii) seam puckering in biofinishing of denim in textile industry. Further pilot plant evaluations, biochemical characterization, and molecular characterization of the cellulase are in progress.

1.2.1.3 Paper biotechnology

Paper recycling industries are oriented towards re-use and sustainability. The major difficulty in recycling of paper is removal of inks. Mixed office waste (MOW) paper includes laser printed and photocopier waste papers coated with toners. These toners are copolymers of styrene and acrylate that get thermally fused with cellulosic fibers of the paper during printing. An alkalistable cellulase from the culture filtrate of an alkalitolerant *Fusarium fusarium* strain was found to be suitable for deinking of MOW papers. The enzyme treatment resulted in the increase in brightness with the reduction in ink counts of the recycled paper.

1.2.1.4 Nano-biotechnology

The encapsulation and immobilization of biological molecules on fatty acid lipid films and nanoparticles has been demonstrated. It has been shown that the encapsulation and interaction of xylanase, from *Thermomonospora* sp., in thermally evaporated fatty amine films by a simple beaker based immersion technique under enzyme-friendly conditions.

Bioconjugation of the nanogold labeled polyurethane microsphere "cores" with the enzyme pepsin leads to a new class of immobilized enzyme material that enjoys the advantage of both the nanoparticle and polymer microsphere-based immobilization methods. Immobilization of *Candida bombicola* cells on standing nanogold membranes and on patterned lipid films as enzyme sources for biotransformation of arachidonic acid to 19 HETE and 20 HETE has been carried out.

Nanoparticles of gold and silver have been synthesized using actinomycetes, *Rodococcus* sp. and *Thermomonospora* sp. The extracellular synthesis of silver nanoparticles by the fungus *Fusarium oxysporum* has been achieved. The gold nanoparticles synthesized by the biological methods have been immobilized in fatty acid and amine thin films. The enzyme involved in extracellular synthesis of nanoparticles by *F. oxysporum,* has been partially purified. The work on the mechanism of synthesis is in progress. The extracellular synthesis of NiS, ZnS, and MnS nanoparticles by *F. oxysporum* has been achieved. Synthesis of Pt, Pd and Cu nanoparticles is in progress.

Biosynthesis of carbonate biominerals using fungi and actinomycetes

Biominerals are essentially inorganic salts, which serve a variety of biological purposes. Laboratory processes for the synthesis of $CaCO_3$ crystals have hitherto relied on very specific proteins from calcareous organisms and an external source of CO_2 for reaction with suitable metal ions. However, these laboratory methods suffer from drawbacks such as being very costly, laborious and give less stable biomineral crystals. Many fungi and actinomycetes are known to release reasonable amount of Co_2 and characteristic proteins during their growth. The advantage of this feature was taken and a novel biological method for the synthesis of $CaCO_3$, $SrCO_3$ and $BaCO_3$ crystals using the whole cell (not pure enzymes) of the endophytic fungus *Vertecillium* sp. which was isolated from *Taxus* plant and plant pathogenic fungus *Fusarium oxysporum* and an actinomycete *Rhodococcus* sp. has been reported. Exposure of the fungal and actinomycete biomass to aqueous Ca^{2+}, Sr^{2+} and Ba^{2+} ion resulted in extracellular synthesis of $CaCO_3$, $SrCO_3$ and $BaCO_3$ crystals of interesting morphology and these truly biogenic crystals showed long term stability also.

Biosynthesis of nanomaterials using medicinal and aromatic plants

The nanoparticles of gold, silver and bimetallic gold core silver shell nanoparticles were prepared by immersing neem and geranium leaves in solution containing chloroauric acid and silver nitrate solution. This has opened up a new and exciting area, as the technique is simple, cheap and environmentally sustainable. It uses no toxic chemicals but only requires geranium and neem leaves and a solution of gold and silver.

1.2.1.5 Secondary metabolites, inhibitors and drugs

Protease inhibitors

An effervescence of research efforts has been expended in the design and synthesis of inhibitors of proteolytic enzymes not only to understand the active site structure and mechanism of these enzymes but also to help generate new therapeutic agents. Specific inhibitors of proteases have proved valuable in a number of applications ranging from mechanistic studies to possible therapeutic uses. Protein inhibitors of proteases are ubiquitously present in plants, animals, and microorganisms. Fundamentally, proteinaceous inhibitors should serve as substrates for proteolysis rather than bring their inhibitors. Elucidation of this paradox is the basis for the extensive research on the structure-function relationship of proteinaceous inhibitors of proteases. The importance of proteolytic processes in the regulation of post-translational processing of precursor proteins and the involvement of proteases in intracellular protein metabolism and in various pathological processes have recently stimulated tremendous interest in studying the kinetic properties of naturally occurring target-oriented protease inhibitors.

Alkaline protease inhibitors

Studies on the kinetics of inhibition of proteinase K by the proeinaceous alkaline protease inhibitor from the *Streptomyces* sp. revealed that the binding is of slow-tight type. The conformational alterations induced in the enzyme are responsible for conferring irreversibility to the enzyme-inhibitor complex.

Aspartic protease inhibitor

The human immunodeficiency virus (HIV), the causative agent of the acquired immunodeficiency syndrome (AIDS) requires the HIV protease enzyme in order to multiply, making this enzyme an excellent target for developing drugs against the virus. The enzyme inhibitors have not only provided effective therapeutic agents for the treatment of diseases but also have led to a detailed understanding of enzyme mechanisms.

An extremophilic *Bacillus* sp. has been isolated, which produces an aspartic protease inhibitor (ATBI). ATBI has been shown to inhibit recombinant HIV-1 protease, pepsin, and the protease from the fungus *Aspergillus saitoi*. ATBI inhibited human pathogens like *Candida kyfer* and *Aspergillus* sp. effectively as seen in the microscopic studies. Based on the amino acid sequence of the natural inhibitor a peptide was synthesized. Currently the potency of the synthetic peptide and the analogues is being evaluated against HIV-1 protease *in vitro*. A few peptidic inhibitors isolated from plant and microbial sources are being characterized.

Cysteine protease inhibitor

Malaria is one of the most prevalent infectious diseases of mankind. Infection caused by the malarial parasite *Plasmodium falciparum* results in the life-threatening complications such as cerebral malaria. Control of malaria is becoming increasingly difficult due to increasing incidence of strains resistant to currently used drugs. The parasitic enzymes which differ structurally or functionally from mammalian enzymes are the rational targets for developing therapeutics drugs. Proteinases play a vital role in the life cycle of the malarial parasite *Plasmodium*. Malarial infection involves an erythrocytic phase where the *Plasmodium* uses a protease, falciparin, for the development of parasite. Blocking of this enzyme is a promising target for new antimalarial drugs. Proteinase inhibitors are, therefore, considered as potential therapeutic agents. Proteinase inhibitors from the broths of the two microbial cultures exhibited a significant growth inhibitory activity against *P. falciparum* in a biological assay based on the inhibition of trophozoite formation.

Drugs

Taxol (Paclitaxel), a natural product initially isolated from Yew tree (*Taxus brevifolia*) is regarded as the most promising anticancer agent. A positive fungal strain which produces side chain ester of Taxol after seven days, 10-deacetylbaccatin (10-DAB) after fourtendays and Taxol after twenty-one days sequentially has been identified. This strain yields 1.5 g/l of Taxol.


Fungus AAT-TS-4

Microbial production of biodegradable plastics

Polyhydroxyalkanoates (PHAs) are biodegradable polyesters and elastomers, which accumulate as cytoplasmic inclusions in certain bacteria during unbalanced growth conditions usually characterized by an excess carbon supply and the lack of one or more essential nutrients. About 150 different hydroxyalkanoic acids have been identified as constituents of bacterial polyesters. Nutritional studies using different carbon source were performed. Glycerol was found to be the best carbon source supporting maximum polyhydroxybutyrate (PHB) accumulation (34.18%) followed by sucrose (28.23%) and molasses (23.06%). The latter could be used as cheaper carbon sources for PHB accumulation. GC analysis and NMR studies confirmed that the accumulated PHA as the homopolymer of PHB when a sole carbon source was used. With the use of glycerol and propionic acid in the medium production of polyhydroxybutyrate-valerate (PHB-HV) copolymer ensured, in which valerate amounted to 50% mol percent of the copolymer. The polymer isolated from *Bacillus sp.* was used for physical characterization studies like NMR, GPC, FTIR, DSC, SEM etc. The polymer was found to be isotactic PHB when *Bacillus* sp. was grown on a single carbon source.

1.2.1.6 Fermentation

An improved process for production of hydrolysing enzyme and alcohol by whole cells of yeast using synthetic zeolites has been developed. Bench scale process has been standardized, which shows 20 - 40% enhancement of fermentation rates compared to the fermentation in absence of additives. At industry site, 100L scale fermentation showed accelerated rates of fermentation with extrudes of zeolites in concentration of 0.07%.

Improving quality and storage stability of *neera*

Neera is produced by tapping the palmyra palm (*Borrasus flabellifer*). it is collected overnight in earthenware pots from an incision made in the inflorescence axis of the spathe and transported under chilled conditions to a local collection centre where it is dispensed to the public as a healthy nutritious drink. It is very popular in the States of Gujarat, Maharashtra, Orissa, West Bengal, Andhra Pradesh, Kerala and Tamil Nadu.

Fresh *neera* has a large microbial population (Bacteria and yeast), due to which it starts fermenting within an hour of its collection. The fermented product, known as Toddy (tadi) is a pungent sour smelling liquid containing 5.0% alcohol. The keeping quality of *neera* is very poor and unless stored under chilled conditions it deteriorates within 5-8 hours after collection.

A laboratory scale membrane filtration technique for removal of bacteria has been developed. The technique is demonstrated to Khadi and Village Industry Commission (KVIC) and the Commission is planning to put up a pilot plant at its *Neera* Processing Center at Dahanu. By using NCL technique, the shelf life of the packaged product can be extended to 10-15 days without affecting the stability, taste and nutrient profile of *neera*.

Gibberellic acid

Gibberellic acid (GA_3) is an important plant growth regulator used in the agriculture, horticulture and brewing. It is a secondary metabolite of fungus *Gibberella fujikuroi*. The product yield is dependent on the strain of the fungus and also fermentation parameters. A selected strain was subjected to UV mutagenesis and a mutant with 25% higher product yield has been successfully obtained. The evaluation of the selected mutant in shake flasks and fermenters has been done and the mutant is now being subjected to subsequent mutations. The fermentation study in 10 L fermenter has shown that there are several key parameters like nutrient quality, temperature, carbon and nitrogen source and oxygen transfer rate that affect the rate of product formation during fermentation. Mutagenesis using UV and EMS will be carried out further for enhanced product yields. The evaluation of strains will be done in 10 L fermenter for optimal production.

1.2.1.7 Process biotechnology

Design and fabrication of a membrane device for production of 95% nitrogen from air used in the controlled atmosphere packaging (CAP) of fruits and vegetables

A membrane based nitrogen generator giving 30 liters/ minute of 95% pure nitrogen used for enhancing the shelf life of fruits and vegetables has been designed and fabricated. The testing of the unit will be carried out at CFTRI, Mysore.

1.2.2 Plant biotechnology

1.2.2.1 Biocontrol and biopesticides

Microbial control of pests: Entomopathogenic fungi as mycoinsecticides

The three promising fungal isolates *Metarhizium anisopliae* M34412, *Beauveria bassiana* B3301 and *Nomuraea rileyi* N812 were compared with the recommended insecticide endosulfan and the biological product HaNPV against *Helicoverpa armigera* on pigeon pea and chickpea under field conditions. The registration trials for the spore formulation of *M. anisopliae* have been carried out at two agriculture universities in Maharashtra and Karnataka.

1.2.2.2 Genetic markers

Molecular approaches to improve the bread making quality potential of wheat

International wheat market follows stringent quality parameters for bread making quality, as wheat is mostly consumed as bread in major part of the world. There is a need to incorporate traits controlling bread making quality in Indian wheat to meet global wheat grain quality criteria for making various end products for domestic and export purpose. Bread making quality (BMQ) is a complex trait influenced by environment and also by gluten proteins (Gliadins and Glutenins) accumulated in the grain. Proportion of gliadin and glutenin, along with the starch content decides the loaf volume.

For this study a recombinant inbred line population (F_{12}) was developed from the cross of HI977 (good BMQ) and HD2329 (high yielding variety with poor BMQ) at Directorate of Wheat Research (DWR), Karnal. Various molecular markers like sequence tagged microsatellite (STMS), inter simple sequence repeats (ISSR), randomly amplified polymorphic DNA (RAPD), amplified fragment length polymorphism (AFLP) were used for parental survey 116 STMS primers (Xgwm) covering most of the chromosomes 800RAPDs and 100 ISSRs were used for screening the parental genotypes. The population is being screened with polymorphic markers to develop a framework map.

Development of leaf and stripe rusts resistant varieties using molecular marker technology

Wheat productivity is severely affected by two important diseases, leaf rust and stripe rust especially in North Western plains of India. Development of agronomically desirable lines with durable resistance to leaf and stripe rust using molecular marker technology is essential to ensure a rust free crop. In order to achieve speedy and reliable incorporation of effective seedling/ adult plant resistance genes, DNA marker(s) linked to such genes need to be employed along with breeding efforts.

Seed material for the parental lines viz. Thatcher, Thatcher + *Lr*-37 (*Lr*-37), CD (*Yr*-16), CDM2D, PBW-343 and UP-2338 along with the Unn WH147 + *Lr*24 (*Lr*24) and Unn WH147 + *Lr*28 (Lr 28) were procured from DWR, Karnal. A set of 100 microsatellite primers procured from University of British Columbia, Canada comprising di-, tri-, tetra- and penta-nucleotide repeat motifs were used for parental screening. In all, 39 primers gave amplification of which 5 primers revealed polymorphism in Tc and Tc+Lr 37 and 2 in CD and CDM2D. Out of 700 random primers (UBC, Canada) used for screening, 175 showed amplification, of which 25 primers revealed 40 polymorphic loci in Tc and Tc+*Lr* 37 and 39 loci in PBW 343 and Tc+Lr 37. Similarly 17 polymorphic UBC RAPD primers revealed 22 polymorphic loci in CD, CDM2D of which 10 loci were recorded to be polymorphic in PBW 343 and CD. Out of 104 microsatellite primer pairs used for screening, 12 showed polymorphism in CD and PBW 343.

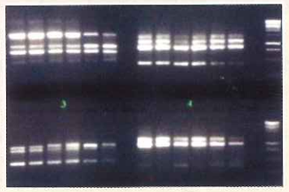
Mapping and tagging of rust resistance genes in wheat

The rusts of leaf, stem and stripe hamper wheat yield. Utilization of genetic resistance, through resistant varieties is the most economical and environment friendly strategy for rust control. A total of 1330 RAPD, 100 ISSR primers and 36 Selective microsatellite primer pairs based on the chromosome location of the genes were screened. One ISSR marker and four microsatellite markers were found to be linked to *Sr9e* and *Sr36*, and formed a linkage group on chromosome 2B, of which ISSR marker UBC 812_{840} and microsatellite Xgwm120 were relatively close with a linkage distance of 14.2 cM and 13.2 cM from *Sr36* and *Sr9e*, respectively. Another ISSR marker UBC 840_{540} was found to be linked to *Lr3a* in repulsion phase at a distance of 6.9 cM. Three microsatellites markers and two RAPD markers were found to be linked to the *Sr22 gene and formed a linkage* Group on 7AL, of which Xgwm573 is relatively close with a distance of 6.4cM.

Development of variety specific markers in mango

India harbors over 1000 varieties of mango. In order to facilitate the mango-breeding programme, these varieties need to be characterized genetically. Marker based DNA fingerprinting is the most obvious mean to proceed with this assignment. In addition, proving the genetic homogeneity of Alphonso clones, which are planted at the largest scale in India, is a major challenge.

Tender leaf tissue of 70 elite varieties of mango were collected from RFRS, Vengurle. Along with this, tender leaf material of 30 Alphonso trees were collected from orchards of three different locations in coastal region of Maharashtra, viz., Dapoli, Deogad and Vengurle. Alphonso collected from different locations were tested for their homogeneity using ISSR markers. Representation of ISSR UBC 810, 811, 813 and 840 marker profiles is shown in the figure.



Another approach is to carry out diversity analysis of mango varieties. ISSR primers were screened using ten elite varieties including Alphonso and one out-group (*Nothopegia sp.*). Screening of ISSR primers is in progress.

Increasing the efficiency of production and nutritional value of chickpea

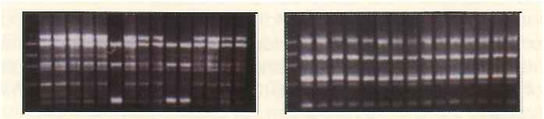
Chickpea, the most important pulse crop of India, is a good source of protein for the primarily vegetarian Indian population. However, average chickpea yield is only 700 Kg /ha, due to its susceptibility to various biotic and abiotic stresses such as Fusarium wilt, Ascochyta blight and drought. Fusarium wilt is a soil borne disease and causes a yield loss of 10-100% annually. Growing resistant cultivars is the most effective strategy to manage the disease. However, identifying / developing resistant cultivars by conventional means is expensive, laborious and time consuming. Molecular breeding would be an effective approach, which involves gene tagging and MAS.

The F9 RIL populations of three crosses (Vijay x JG 62, JG62 x ICC 4958 and Vijay x ICC 4958) were raised at MPKV Rahuri and wilt data were collected from sick plots. Agronomic data and the leaf tissue for DNA analysis of the RILs were collected from normal plots. 100 ISSR and 100 STMS primers were used for parental analysis, of which 15 ISSR and 23 STMS primers were polymorphic. Currently, analysis of the Cross-III RILs is being done with the polymorphic primers. Diversity Analysis of wild chickpea germplasm with RGA markers is also being done.

DNA based quality control of plants

The clonal fidelity and uniformity of the micro propagated plants is a major concern of tissue culture industry as well as of the farmers. The variation within the progeny results in serious losses to the end users, thus making quality control of tissue culture (TC) raised plants mandatory. The objectives of the project are to develop fingerprints for the mother plants and clones of the identified plant species (Banana, Eucalyptus, Teak etc.) using PCR based markers and to test quality of TC raised plants.

Molecular analysis of TC raised Teak plants was done with the set of 100 ISSR primers and 800 UBC RAPD primers. Customer service for Date palm fidelity has been done. ISSR analysis of TC raised plants of bamboo, ginger and turmeric was also carried out.



Fidelity analysis of turmeric and ginger plants using ISSR Primer

Improved productivity, profitability and sustainability of sheep production

Sheep constitutes an important species of livestock in the rural agricultural economy of arid and semi arid zones in India. The major factors contributing to the low productivity of sheep include poor exploitation of genetic potential of indigenous animals, insufficient resources of feed, fodder and health cover and inadequate efforts to improve sheep breed. It is thus important that the sheep breeding be strengthened through genetic improvement of local breeds and improvement of nutrition management and health care.

Almost all Indian sheep breeds are non prolific except Garole, which carries the prolificacy gene (FecB). Hence, to increase the prolificacy of Deccani, the main meat type sheep breed of Maharashtra, crossbreeding between the Garole and Deccani was carried out. The introgression of the prolificacy gene in prolificacy flocks developed was studied with the help of PCR RFLP test. Introduction of one copy of the gene increased the ovulation rate by 0.6 and litter size by 0.5 in Deccani. Such a moderate increase in the prolificacy is suitable for the sheep rearing conditions in Maharashtra.

The sheep breeds, Deccani, Patanwadi, Marwadi, Madras Red, Bannur and Garole, representing various advantageous traits are being studied for genetic diversity. A molecular marker set spanning different chromosomal regions of sheep genome is being used to analyze the genetic diversity. Such data will be helpful in planning the breeding programs for the strain improvement by pyramiding desired characteristics such as high prolificacy, adaptability to harsh environments, disease resistance, good body conformation for meat purpose and producing good quality wool.

1.2.2.3 Host-pathogen interactions

Transcript profiling during host-pathogen interactions with reference to chickpea and *Fusarium oxysporum* f. Sp. ciceri

Wilt caused by *Fusarium oxysporum* f.sp. ciceri (FOC) is an important disease of chickpea leading to heavy losses. Seven races of FOC are known world wide, of which race 1 and 2 are prevalent in central India. Although excellent resistant plant sources are available in chickpea germplasm, success in breeding for FOC-resistance is limited, mainly due to region-specific races of FOC and gradual breakdown of resistance in chickpea cultivars. Molecular mechanisms involved in chickpea-FOC interactions are being explored by analyzing root cDNA libraries in established resistant (WR 315) and susceptible (JG 62) cultivars in response to FOC-race 1. Next set of 8 primer pair combinations was tried out for cDNA-AFLP. Totally 39 transcripts were identified as differentially expressed/ upregulated in the resistant infected root library and were purified from the gel and reamplified and cloning of these transcripts into pGEMT-Easy vector is in process. The clones will be further used for DNA sequencing. Probable genes active during the host-pathogen interaction, WRKY proteins, 14-3-3 proteins and LRR type sequences have been identified. Isolation of full-length cDNA from the library of these genes with a putative role in host-pathogen interactions is being carried out.

Development of race specific marker

Race 1, 2 and two representative isolates of each race. AFLP primers, which showed polymorphism for race 1, 2 and their isolates, have been used for this study. Polymorphic bands of size ranging from 100 400 bp were obtained. These polymorphic bands were eluted from 6% denaturing PAGE gels, re- amplified, precipitated and then cloned into pGEMT vector (Promega). The presence of inserts was determined by M13F/R amplification. Some of these clones have been sequenced. The sequencing data will be used to design primers for developing a race specific marker.

Identifying virulence genes in *Fusarium*

Homology search of the sequences of the polymorphic bands revealed that one of the bands shows homology to *Fusarium oxysporum* f.sp. *Melonis* transposon Hop78. Studies showed that transposons are related to the pathogenicity of fungi. Primers towards the conserved regions of known virulence genes of different fungal genera have been designed. These primers will be used to locate the corresponding virulence genes in *Fusarium*.

1.2.2.4 Transgenic plants

Gene transfer technology allows the transfer of genetic information from one organism to another regardless of the sexual compatibility of the two organisms. A transgenic plant contains genes which have been inserted into a plant either by microprojectile bombardment, Agrobacterium mediated gene transfer or by electroporation method.

Development of transgenic plants *Curcuma longa and Pinus roxburghii*

Transformation work is initiated for *Curcuma longa* (Turmeric) and *Pinus roxburghii*. An efficient plant regeneration system of the desired plant sp. is a prime requirement for any of these genetic transformation methods. Different plant organs were used to produce callus mass or direct organogenesis by growing them on defined media. The hormonal and other chemical requirements of the growing tissue were standardized along with physical parameters such as light and temperature for organogenetic response. The protocol was also standardized for acclimatization of the plantlets regenerated from this system. Genetic transformation work was then undertaken after standardizing the regeneration system in both the plant species. The study of transient expression of the gene gave promising results. Further DNA analysis such as PCR and southern hybridization is in progress.

Winged bean proteinase inhibitor for *Helicoverpa armigera* resistance

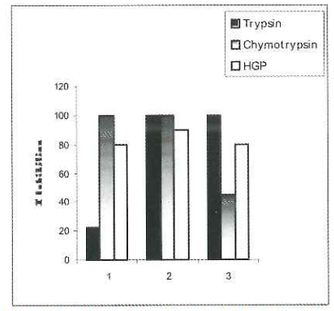
H. armigera, pod borer, is a serious insect pest of over 100 different plant species including many important crops such as cotton and tomato, and the legumes like chickpea and pigeon pea. Among the numerous biomolecules that could potentially be utilized in enhancing plant defense against insect pests, *Bacillus thuringiensis* (Bt) toxins represent the most extensively used example of biopesticides, and a few transgenic crop plants expressing Bt genes have seen commercial use. However, persistence of Bt toxins within the plant throughout the growing season is likely to induce a widespread resistance to Bt in insects in the near future and this has necessitated the search for newer and more effective biological means of controlling insects. Among the various alternatives to Bt, proteinase inhibitors (PIs) represent an attractive class of biopesticides and exhibit several important features.

PIs from a number of species have been screened and it has been demonstrated that the pooled PIs from seeds of winged bean (WB), which is a non-host plant of pod borer, inhibit the *H. armigera* gut proteinases (HGPs) and pod borer larval growth. Dry mature seeds of winged bean contain several proteinase inhibitors. Two-dimensional gel analysis of WB seed protein followed by activity visualization using a gel-X-ray film contact print technique revealed at least 14 trypsin inhibitors (TIs) in the range of 28 to 6 kD. A total of seven inhibitors (WBTI-1 to 7) were purified by heat treatment and gel filtration followed by elution from preparative native gels. Based on their biochemical characterization such as molecular mass, pI, heat stability, and susceptibility to inactivation by reducing agents, WBTI-1 to 4 are Kunitz type inhibitor while WBTI-5 to 7 are classified as Bowman-Birk type serine proteinase inhibitors. Although Kunitz type TIs (20-24 kD) of WB have been reported, the smaller TIs that belong to the Bowman-Birk type have not been previously characterized. Seven major TIs isolated from WB seed were individually assessed for their potential to inhibit the HGP of WBTI-1 (28 kD) was identified as a potent inhibitor of HGP relative to trypsin and among the all other WBTIs; it inhibited 94% of HGP activity while at the same concentration it inhibited only 22% of trypsin activity. WBTI-2 (24 kD) and WBTI-4 (20 kD) inhibited HGP activity above 85%. WBTI-3, -5, -6 and -7 showed limited inhibition of HGP as compared with trypsin. These results indicate that WBTIs have different binding potentials towards HGP although most of the HGP activity is trypsin-like. A simple and versatile method for identifying and purifying PIs after two-dimensional separation using the gel-X-ray film contact print technique has been developed.

Isolation and cloning of winged bean proteinase inhibitor genes in expression vector

Winged bean seeds have been identified as potential source of proteinase inhibitors possessing insect anti-digestive activity. Next logical step in this project was to isolate inhibitor genes from winged bean, express in model organism and test their potential against target insect *Helicoverpa armigera*. Winged bean (*Psophocarpus tetragonolobus* L. DC.) chymotrypsin inhibitor (PtWCI) genes have been characterized earlier for their sequence analysis and *in vivo* expression in winged bean plants.

On the available database sequence information, primers from flanking regions of PtWCIs to isolate respective gene have been designed. Cloning of four PtWCIs in *E. coli* expression vector (pCRT7/NT TOPO, 3.0 kb) has been successfully achieved. However, expression level was too low in *E. coli* strain BL21 DE3 cells as these gene products are toxic to the cells. Therefore, use of *Pichia pastoris* as expression system for secreted expression has been planned.



Inhibition of trypsin, chymotrypsin and HGP by recombinant WBPIs

The work on (i) sequence analysis of isolated winged bean proteinase inhibitor genes (ii) cloning of winged bean proteinase inhibitor genes in *P. pastoris*.expression vector pPIC9 under AOX1 promoter (iii) transformation of selected PtWCI clones in to *P. pastoris* and (iv) cloning of PtWCIs in binary vector under tissue specific promoter has been carried out.

Bitter gourd proteinase inhibitors: potential growth inhibitor of *Helicoverpa armigera* and *Spodoptera litura*

Since *H. armigera* gut proteinase are very flexible in expression and possesses molecular diversity in serine proteinase family encoding 28 different genes, the possibilities to find potential

proteinase serine inhibitors of all the four subtypes found in plants are being explored. Bitter gourd seeds contain squash type proteinase inhibitors having a smallest protein proteinase inhibitor with very binding capacities. The objective of the project is to isolate and characterize bitter gourd proteinase inhibitor and test their potential against *H. armigera*.

Proteinase inhibitors (PIs) from the seeds of bitter gourd (*Momordica charantia* L.) were identified as strong inhibitors of *H. armigera* gut proteinases (HGP). Biochemical investigations showed that bitter gourd PIs (BGPIs) inhibited more than 80% HGP activity. Electrophoretic analysis revealed the presence of two major proteins (BGPI-1 and -2) and two minor proteins (BGPI-3 and -4) having inhibitory activity against both trypsin and HGP. The major isoforms BGPI-1 and BGPI-2 have molecular mass of 3.5 kDa and 3.0 kDa respectively. BGPIs inhibited HGP activity of larvae fed on different host plants, on artificial diet with or without added PIs and proteinases excreted in fecal matter. Degradation of BGPI-1 by HGP showed direct correlation with accumulation of BGPI-2-like peptide, which remained stable and active against high concentrations of HGP up to 3 hours. Chemical inhibitors of serine proteinases offered partial protection to BGPI-1 from degradation by HGP, suggesting that trypsin and chymotrypsin like proteinases are involved in degradation of BGPI-1. In larval feeding studies, BGPIs were found to retard growth and development of lepidopteran pests namely *H. armigera* and *Spodoptera litura*. This is the first report showing that BGPIs mediated inhibition of insect gut proteinases directly affects fertility and fecundity of both *H. armigera* and *S. litura*. The results advocate use of BGPIs to introduce insect resistance in otherwise susceptible plants. Further, two partial bitter gourd PIs genes were isolated by using the primers designed from N-terminal sequence of protein. These DNA fragments were cloned and sequence characterized.

Purification of capsicum proteinase inhibitors and their interaction with insect gut proteinases

Capsicum has wound inducible proteinase inhibitors (PIs) present in their leaves as well as in other plant parts. The objective is to identify and characterize all four types of plant proteinaceous serine proteinase inhibitors which have strong potential against insect gut proteinases.

Capsicum PIs were purified by DEAE Sepharose FAST FLOW ion exchange and gel filtration columns. All the capsicum PIs were precipitated at 65% of ammonium sulphate and their thermal stability (up to 65°C) Allowed to use thermal denaturation step to remove non-inhibitor proteins. Specific trypsin inhibitor activity of capsicum PI extract was increased by four folds after these two steps. Two major peaks of inhibitor *cap*A1 and *cap*A2 were observed in the buffer (50mM Tris-HCl, pH 7.8) wash. Remaining isoforms of *cap* PI were eluted out in fine step gradient of NaCl. Cap B2 was eluted out at 0.25 M NaCl as a single inhibitor protein while other three forms of PI were resolved in three different mixtures like *cap*B2+*cap*C, *cap*C+*cap*D+*cap*E, *cap*D+*cap*E at slightly different molar concentrations of NaCl. Elution of three cap PI isoforms *(capC, capD, capE)* in different mixtures and almost at similar salt concentrations indicates similarity in their charge and mass properties. Two major inhibitor activities *cap* PIs, *cap*A1 and *cap*A2, were selected for further purification. Pooled fractions of *cap*A1 and *cap*A2 were reloaded on DEAE matrix, which eliminated the non inhibitor proteins completely except one high molecular protein of ~96 kD, which was subsequently eliminated by rechromatographing on sephadex G-75 gel filtration column.

Chickpea proteinase inhibitors in defence against *Helicoverpa armigera*

Chickpea (*Cicer arietinum* L.) is the major source of dietary proteins for the majority vegetarian Indian population. Chickpea crops face immense losses every year due to the combined action of biotic stresses like insect and fungal attack. The Pod borer (*H. armigera*) is a devastating insect pest that is known to attack and infest about 180 different plant species including chickpea. Efforts are on to identify, characterize and employ defensive genes in transgenic programmes to develop insect resistance in chickpea. Currently, *Bacillus thuringiensis* Endotoxin (Bt), proteinase inhibitors (PIs), amylase inhibitors and lectins are the most successful and promising candidates.

H.armigera gut proteinose inhibitor (HGPI) protein was purified to homogeneity from dry and mature seeds of chickpea using conventional methods i.e., gel-filtration and ion exchange chromatography. molecular weight was determined to be ~21kDa. iso-electric point was predicted to be around 5.90. purified protein was identified by n-terminal 20 amino acid sequencing as well as by matrix associated laser desorption ionization-time of flight (maldi-tof) spectrometry.

From the available protein & gene sequences, oligonucleotide primers were synthesised and used in a polymerase chain reaction (PCR) for amplification of gene which was then sequenced by flouroscent automated sequencing. This gene was directionally inserted into the plasmid pgapzαb, which is a vector specifically constructed for heterologous gene expression in the yeast *pichia pastoris*. Positive yeast clones (carrying hgpi gene) were isolated and expression of hgpi protein confirmed by western blot hybridization.

Large-scale yeast-expression of HGPI protein was carried out in a 2000 ml capacity bio-fermenter and pure recombinant protein obtained (~25mg per fermenter run). *In vitro* assays have revealed that the purified as well as recombinant (expressed) inhibitors have comparable stability and inhibitory activity against bovine trypsin and HGP.

Tomato proteinase inhibitors and their interaction with *Helicoverpa armigera* gut proteinases

Tomato PIs are wound inducible, their level of expression increases 5-10 folds if a plant leaves are damaged or attacked by the insect pests. *H.* armigera feeds on young foliage and developing fruits but not on flowers. Different tissue of tomato plants for qualitative and quantitative differences in proteinase inhibitors were analysed.

The extracts of different tissues were made using 5mM EDTA, 20 mM EDTA, 1M KCl followed by 70% $(NH_4)_2SO_4$ precipitation, dialysis and heat Treatment at 70°C. The protein was quantified using Bradford's method. Extracts were analyzed for inhibition potentials against trypsin, chymotrypsin and several HGPs, including HGP of larvae fed on chickpea, pigeon pea, sweat pea, okra and tomato which are host plants and of larvae fed on artificial diet containing the proteinase inhibitors of non-host plant viz. winged bean and potato Pin II. The extract was also assayed against HGP of different larval instars. Proteinase inhibitor profiles in all the plant parts are identical exhibiting four isoforms. However, the amount of inhibitor significantly varies in different tissue and very high (100-500 fold more) in flower as compared any other tissue type. Therefore, study was concentrated on tomato flower PIs which shows ≥75 % inhibition of HGP of host fed larvae while it shows ≥70 % inhibition of HGP of non-host fed larvae. Based on all the results it is seen that tomato proteinase inhibitors are strong inhibitors of HGP. Therefore, thorough analysis of this endogenous defense source could help in solving the problem of *H. armigera* attack on tomato. Work on standardization of tomato regeneration protocol to perform transformation experiments with winged bean proteinase inhibitor genes has been initiated.

Expression studies of *H. armigera* gut proteinases for the identification of proteinase inhibitor insensitive proteinases

H. armigera has developed an ability to overcome the adverse effects of proteinase inhibitors (PIs), which is being used to produce insect tolerant transgenic crop plants. The PI overcoming mechanism is mediated by larval gut proteinases. Therefore identification of such proteinases genes and their function in terms of sensitivity to various inhibitors is very much essential. This would help in identification and/ or design of effective PIs for their deployment in crop plant defense.

Proteinase specific primers were designed from the available sequences of trypsin-like, chymotrypsin-like, carboxy and aminopeptidase-like, elastase-like, cathepsin-like proteinases. These primers were used for quantitative expression analysis of gut proteinase using RT-PCR. Total RNA from the insect gut fed on host plants (chickpea, cotton, pigeonpea, tomato, okra) and non-host PIs (winged bean, capsicum bitter gourd and groundnut) was used for the study. This analysis enabled us to point out some trypsin-like and chymotrypsin-like proteinase genes, which may have role in PI insensitivity. Isolation of full-length genes of these proteinases using RACE-PCR is in progress.

1.2.2.5 Secondary metabolites

Biomolecular prospecting of *Symplocos* and *Gaultheria* species

Biodiversity is of prime importance and rigorous efforts are needed to conserve and maintain the genes, species and ecosystems for the sustainable use and management of biological resources. In light of this, genetic diversity directed conservation would be a better proposition to be adopted The present study is an effort to understand the status of genetic diversity present in two plant species, *G. fragrantissima* and *S. laurina*, from two biodiversity hotspot regions in India. In the present study molecular markers have been used to study the genetic diversity in *G. fragrantissima* from the two hotspots in India.

PCR- RFLP technique was used to study chloroplast and mitochondrial DNA diversity in *G. fragrantissima*. Nine cpDNA and seven mtDNA haplotypes have been detected from eight populations. Variations in the yield of oil and content of methyl salicylate were studied in relation to the season of collection of leaves and the geographic location of the plants. Collection tours are being carried out for *S. laurina*.

1.2.3 Plant tissue culture

1.2.3.1 Tissue culture

Induction of downy mildew resistance in commercial cultivars of grapes

This is a multi-institutional project between NCL, Agharkar Research Institute (ARI), Pune and National Research Centre for Grapes (NRCG), Pune. Due to importance of grape cultivation in India and the adverse affects of fungus diseases on grapes, the programme was undertaken with the prime objective of development of downy mildew resistant varieties of Thompson seedless and Flame seedless by conventional breeding and embryo rescue methods. The project also aimed to characterize hybrid nature of seedlings and to assess the diversity of the wild species of grapes native to India, through DNA marker technology. Using breeding and *in vitro* embryo rescue methods, about 500 hybrid plants of Thompson seedless and Flame seedless (both used as female parents) crossed with 8 downy mildew resistant parents (used as male parents) have been developed. These plants have been supplied to NRCG for further field evaluation.

Tissue culture studies in medicinal plants

The project entitled "Assessment and *in vitro* conservation of biodiversity in some *Guttiferous* plant species of Western Ghats with special reference to the development of bioactive molecules" is sponsored by Department of Biotechnology (DBT), New Delhi. Among the eleven genera of medicinal importance from the family Guttiferae, four are endemic to India. The genus *Calophyllum* is represented in India by fourteen species. Out of which four species are endemic to Western Ghats.

The objective of present project is to evaluate the status of distribution, chemotaxonomic analysis and to generate *in vitro* regeneration protocols. The other objectives are to evaluate new natural compounds, isolate and to study variation among different species/ habitats. About twenty-five accessions were collected from different locations from some districts of Maharashtra and Karnataka. Standardization for in vitro regeneration using different explants for three species of *Calophyllum* is being carried out.

1.2.3.2 Micro-propagation

Under this project from Department of Biotechnology, technologies are being developed for micropropagation of

Casuarina, Accacia and *Pinus*. The upscaling of micropropagation technologies already developed for *Eucalyptus palita*, ginger, turmeric, *Centella* and some ornamental as well as medicinal plants is going on.

For social forestry programmes teak, *Eucalyptus* and bamboo are being multiplied. The germplasm of important plant species is being maintained.

Under the project sponsored by Ministry of Health and Family Welfare, Government of India the micropropagation protocol is being developed for the medicinal plants namely: *Chlorophytum borivilianium, C. arundinaceum, Rauwolfia serpentina,* and *Swertia chirata.*

Micropropagation of selected grape varieties and rootstocks and DNA fingerprinting of germplasm

This is a multi-institutional project between NCL, Agharkar Research Institute (ARI) and National Research Centre for Grapes (NRCG), Pune. The main objective of the programme at NCL is to develop and refine *in vitro* plant regeneration protocols of selected rootstocks and varieties of grapevine. Four varieties (Red globe, 2A Clone, Crimson Seedless and Italia) which are of commercial importance and two rootstocks (110R and 1103P) which have tolerance to drought and salinity were selected for micropropagation studies. Aseptic cultures of all the varieties and rootstocks, initiate shoots, induce multiple shoot formation, elongation of shoots, induction of *in vitro* rooting of shoots, hardening of plants have been established. Tissue culture plants, number in brackets: Red Globe (555), 2A-Clone (396), Crimson Seedless (96), 110R (15) and 1103P (14) have been produced. These plants after hardening in plastic cups have been supplied to NRCG for further planting in the field for evaluation and multiplication.

Micropropagation and germplasm conservation of endangered medicinal plants of Western Ghats

Gymnema sylvestre and *Bidaria khandalensis* are medicinally important woody climbers. *G. sylvestre* is well known in traditional medicine for diabetes mellitus and stomachic. *B. khandalensis* is inhibitor of glucan synthesis and it prevents dental plaque. *Iphigenia magnifica* is another valuable medicinal plant.

G. sylvestre and *B. khandalensis* nodal segment cultured in MS medium supplemented with different phytohormons showed varied responses. The axillary buds from the explants sprouted and grew in length on a majority of the media. However, in presence of BAP and NAA in the medium, multiple shoots were regenerated. The regenerants were allowed to grow and later excised and transferred to the rooting medium containing IBA. Attempts are in progress to harden the regenerants.

The corms of *I. magnifica* were sliced and cultured on MS medium supplemented with a combination of BAP and kinetin. The dormant buds regenerated up to a maximum of two shoot per slice. The regenerants were allowed to grow on the same medium where these formed corm and roots while still attached to the mother explant. The fully developed plants were detached from the mother explant and transferred to fresh medium for further growth. Individual plants were transferred to pots for hardening. Attempts are in progress to enhance the regeneration ratios and harden the plants under green house conditions so that these could be out planted.

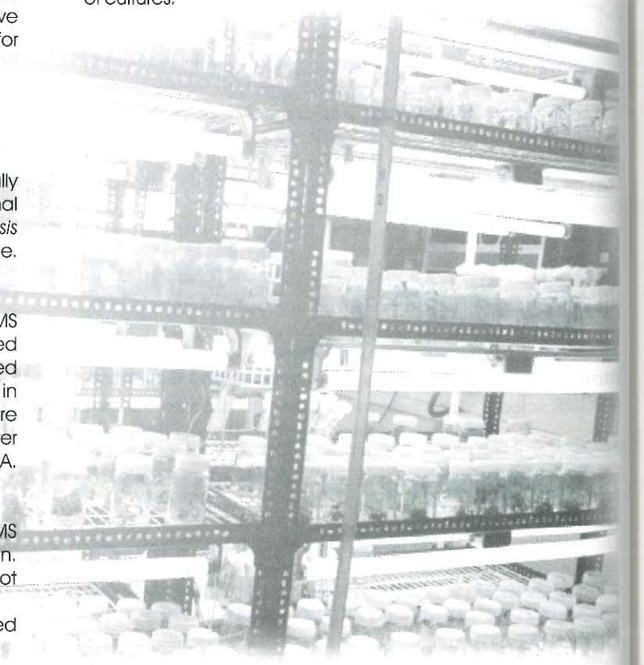
In vitro morphogenesis and genetic transformation in peanut

Plant transformation requires a good regeneration protocol. Extensive work has been carried out on *in vitro* regeneration of peanut from various explants via organogenesis and embryogenesis and a lead in the area of peanut tissue culture has been established. The available protocols are extremely reliable and appropriate for both genetic transformation and for morphogenetic studies.

1.2.3.3 Embryogenesis

Somatic embryogenesis in cashew and mango

Somatic embryogenesis in cashew was obtained from nucellar tissue from immature fruits and immature zygotic embryos. Histological studies revealed that superficial cells of embryogenic callus gave rise to somatic embryos. Experiments are being carried out for successful conversion of somatic embryos to plantlets. Similar work is also done for mango sp. The somatic embryogenic cultures of cashew and mango are used for mutant development programme using radiation technology under IAEA Project. These cultures are also used to develop cryopreservation technique for long term preservation of cultures.



2. Catalysis

2.1 Heterogeneous catalysis

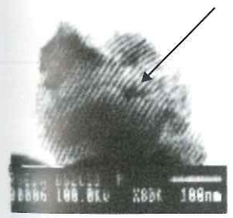
2.1.1 Catalyst: Microporous and mesoporous materials

2.1.1.1 Microporous and mesoporous metallosilicates

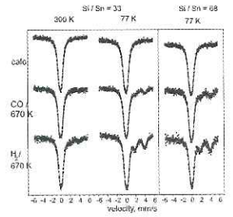
Zeolite beta is very important commercial catalyst mainly used in alkylation and acylation of aromatics. It was synthesized using fly ash as a combined source of SiO_2 and Al_2O_3. In this method, fly ash which is obnoxious by-product of thermal power plants can be used to produce high value and high performance catalysts. Using the concept of promoters in zeolite synthesis, three new zeolite structures of beta family were obtained.

Siliceous mesoporous MCM-41 and SBA-15, synthesized by the supramolecular templating approach using alkyl trimethyl ammonium halide (e.g, CTMABr) and block co-polymers (e.g, P123/P103) as the structure directors in basic and acidic conditions, respectively, relies as a novel support surface for the introduction of active metal/ organometallic species (V-MCM-41, Ti-MCM-41, V/SBA-15, etc) because of its variable internal pore diameter, large surface area and abundant silanol sites.

Incorporation of tin in SBA-15 using two different metal sources has successfully demonstrated that tin oxide exists as a thin film anchored inside the mesopores of SBA-15 due to the reaction of the abundant surface silanol groups with the Sn precursor. The two types of Sn species identified are i) the one stabilized atomically (well dispersed Si-O-Sn-O-Si- groups) on the walls,



TEM of Sn-SBA-15
(arrow mark shows Sn)



Mössbauer spectra
Sn-SBA-15 of samples

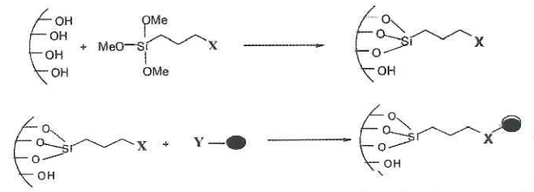
which form Sn^{2+} upon reduction treatment (easily reducible from Sn^{4+} to Sn^{2+} in presence of OH groups) and ii) the large size entities $Sn^{4+}(SnO_2)$ clusters distributed in the external pore structure, which are seen by TEM and are probably agglomerates of smaller crystallites (XRD data). These samples are effective in catalyzing the transesterification of a diketo ester.

2.1.1.2 Mesoporous carbon

Mesoporous carbon material is prepared by using silica based mesoporous materials like MCM-41 or SBA-15 as base material. Mesoporous MCM-41 or SBA-15 was made in the laboratory by standard procedure. Thereafter it was mixed with calculated amount of sucrose, followed by heating at ~150°C. the procedure was repeated to get black material. Finally the material was calcined at ~1000°C followed by washing with hydrofluoric acid and drying at 110°C. The resulting mesoporous carbon material showed that the surface area was around 900 $m^2 gm^{-1}$, the pore diameter was 3.7 nm, pore volume was 0.84 cc/gm) and the TEM showed hexagonal channels.

2.1.1.3 Mesoporous organo-inorganic hybrid heterogeneous chiral catalysts

The unique features of these mesoporous materials can be well utilized for the synthesis of novel organic-inorganic hybrid mesoporous materials using various organosilanes having active donor sites (-NH_2, -Cl, -SH, -$(PPh_3)_3$, -OH), by in situ method or by post synthesis grafting methods, for the heterogenization of various active metal complexes /chiral metal complexes. Thus, the heterogenization of useful homogeneous catalysts over hybrid mesoporous materials having active donor sites finds improved catalytic properties than the conventional amorphous silica supported metal catalysts, due to the periodicity in the pore walls which in-turn inhibits the mass transfer related problems and hence is less prone to deactivation resulting in a higher level of productivity.



X= -Cl, -NH_2, -SH & Y belongs to chiral moiety / metal complex

The evidence for the presence of close-packed conformation of aminopropyl or thiol carbon chains can be obtained from the ^{29}Si MAS NMR of NH_2- or SH-propyl-MCM-41 samples. While the two peaks at about -101 and -111 ppm are attributed to Q_3 and Q_4 species for siliceous MCM-41 respectively, the three peaks at about -50, -60 and -67 ppm are assigned to isolated, terminal and cross-linked siloxane groups attached with pendant aminopropyl groups, respectively. The peak intensities of different siloxane groups are in the order: isolated < terminal < cross-linked.

2.1.2 Catalysis

2.1.2.1 Petrochemicals

Low temperature, solvent-free liquid phase isopropylation of aromatics

Isopropylation of i) benzene to cumene, ii) ethylbenzene to ethylcumenes, and iii) xylenes to dimethyl-cumenes was studied. HX formed (scheme below) can be reacted to propylene and hence recycled *in situ*. Iron and gallium-containing zeolite beta, USY and ZSM-5 samples were prepared and characterized. To study the effect of poisoning of external surface of these catalysts on catalytic activity and product selectivity, special technique was used to selectively passivate the non-shape selective external surface. These catalysts will be tested solvent-free, low temperature ring isopropylation of benzene to cumene and di-isopropylated benzene using alkylhalide as alkylating agent as shown in the table.

For benzene R = R_1 = H, for toluene R = CH_3 and R_1 = H, for xylenes R = R_1 = CH_3 and for ethylbenzene R = C_2H_5 and R_1 = H.

Effect of exchange cations in zeolite beta

Catalyst	Time (min)	2-BP Conv (mol.%)	Cumene (mol %)	DIPB, (mol %)	DIPB Distribution (mol.%)		
					1,2-DIPB	1,3-DIPB	1,4-DIPB
Fe/Beta	100	100	85.8	14.2	0.0	34.5	65.5
Ga /Beta	180	100	85.5	14.5	0.0	42.9	57.1
Cu/Beta	840	31.90	98.9	1.1	0.0	29.1	70.9
Zn/Beta	840	15.2	96.6	3.4	0.0	33.8	66.2

Reaction conditions: substrate: benzene; alkylating agent: 2-bromopropane; benzene: 2-bromopropane (4:1) mole/mole catalyst: 0. 2 gm; temperature: 80°C

The liberation of HX is drawback in this whole process for commercial exploitation; however, this challenge is surmountable as there is hardly any moisture present in the system.

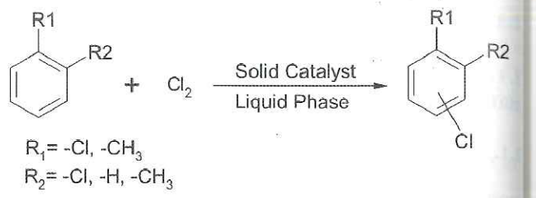
2.1.2.2 Fine chemicals

2.1.2.2.1 Solid acid catalysts

The work was carried out on replacement of environmentally hazardous homogenous acid catalysts like mineral acids ($AlCl_3$, $FeCl_3$, etc.) by eco-safer solid catalysts. Some examples of the work done using solid catalysts are:

Chlorination of aromatics

The liquid phase selective para-chlorination of aromatics such as chlorobenzene to para-chlorobenzene, ortho-dichlorobenzene to 1,2,4-trichlorobenzene, toluene to para-chlorotoluene (pilot plant scale is successfully demonstrated) and o-xylene to 4-chloro-o-xylene has been carried out using recyclable, solid, para-selective and environment friendly catalysts. The selective para-chlorination of these compounds is significant from the industrial point of view. The most important product, para-chlorotoluene is used as an intermediate in the pesticide, pharmaceutical, peroxide, dye and other industries. The production of 4-chloro-o-xylene in high selectivity is important due to its usefulness in the production of intermediates for thermoplastics, pharmaceuticals and agrochemicals.

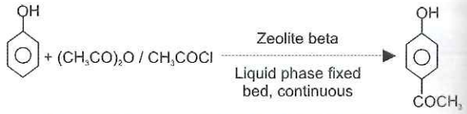


R_1= -Cl, $-CH_3$
R_2= -Cl, -H, $-CH_3$

Acylation of aromatics

Selective acylation of aromatics is of considerable interest due to its commercial importance in several organic intermediates for the production of fine chemicals. The difficulties encountered with homogeneous catalyst systems and for environmentally clean process, the solid, selective and recyclable catalysts have been developed for the acylation of aromatics. The acylation of aromatic substrates is of considerable interest for making intermediates which are widely used for the production of pharmaceuticals, perfumes, dyes and insecticides. The liquid phase selective acylation of aromatics such as toluene to 4-methylacetophenone, anisole to 4-methoxy acetophenone (4-MAP), veretrole to 3,4-methoxypropiophenone, chlorobenzene to 4,4'-dichlorobenzophenone and biphenyl to 4-phenylbenzophenone has been carried out using solid catalysts like zeolite (e.g, zeolite beta) and acetic anhydride or acetylchloride as acylation reagent.

A bench scale process for the preparation of 4-MAP using H-beta zeolite has been developed.



Schematic representation of preparation of 4-MAP using H-beta zeolite

2.1.2.2.2 Vapour phase nitration and oxidation of aromatics

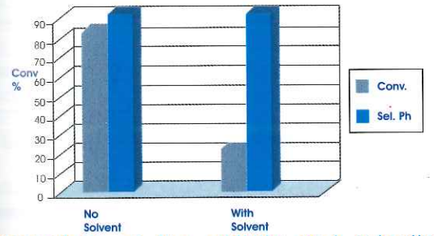
Direct nitration of benzene to nitrobenzene using dilute HNO_3 as nitrating agent and solid oxide based catalyst has been achieved. A simple fixed bed continuous process has been successfully developed at bench level scale. The new process is based on heterogeneous catalysis where nitric acid and benzene vapours are passed over solid acid catalyst without any use of sulphuric acid and hence it is an environment friendly process. A solid acid catalyst of high acidity (superacid catalyst) has been developed with a high surface area and tested for 200 hours which showed high conversion of nitric acid (>80%) and high selectivity (>99.7%) for mono-nitrobenzene. Use of solid acid catalyst, which showed long life, good conversion and selectivity for nitrobenzene, has following advantages over conventional H_2SO_4 process.

- No use of sulphuric acid (conventional process) and hence no disposal problems,
- Less by-product formation with 99.7-100% product purity, and
- Ease of operation: Vapours of benzene and nitric acid are passed over solid acid catalyst in a down flow reactor and the product is collected at the outlet.

2.1.2.2.3 Liquid phase heterogeneous oxidation

Solvent-free direct hydroxylation of aromatics

Direct hydroxylation of aromatics like benzene, toluene, phenol, anisole, etc. and olefinic compounds using solid catalysts and dilute hydrogen peroxide is of great importance in developing eco-friendly processes for industrially important phenolics and epoxy compounds. The major drawback of the liquid phase heterogeneous catalysis is the common use of a co-solvent, which poses various down stream problems like solvent loss during separation and solvent recovery. Additionally, the use of organic solvent is not recommended from green chemistry approach. Hence, a programme was taken up for direct hydroxylation of aromatics using solid TS-1 as catalysts and very dilute H_2O_2 using water as reaction medium in the absence of any organic solvent. The aromatics studied were benzene, toluene, anisole and phenol. The salient results in the hydroxylation of benzene are depicted graphically.



Comparison of the activity and selectivity in the presence and absence of organic solvent using water as reaction medium, TS-1 as solid catalysts and dilute H_2O_2.

Chemoselective epoxidation of olifinic compounds

The epoxidation of various olifinic compounds like styrene, ally chloride, allyl alcohol, methallyl alcohol and methallyl chloride using solid zeolite catalysts and dilute hydrogen peroxide was carried out under liquid phase conditions. The salient features of allylic substrates are tabulated below:

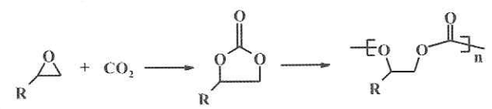
Comparison of the chemoselective epoxidation of allyl and methallyl substrates

Substrate	Temp., (K)	Conv., %	Selectivity, %			
			epoxide	aldehyde	acid	others
allyl alcohol	323	65	96	4.0	-	-
allyl chloride	323	90	95	-	10	5
methallyl alcohol	333	62	72	12	-	6
methallyl chloride	333	72	90	-	-	10

The conversion of allyl/ methallyl chloride is higher than the corresponding alcohol under similar reaction conditions. It is expected that the greater electronegativity/ electron withdrawing character of O vis-à-vis Cl will deactivate the adjacent C=C bond, as observed.

2.1.2.2.4 CO_2 utilization

Utilization of CO_2 as C_1-feedstock in chemicals and fuels synthesis is of great interest. Among the various CO_2-based reactions the coupling of CO_2 with i) epoxides yielding cyclic and polycarbonates (scheme 1) and ii) primary amine and alkyl halides yielding the corresponding carbamates (scheme 2) are important as they are the most efficient ways of CO_2 utilization. Moreover, the products (cyclic carbonates and carbamates) are highly valued-chemicals and are used in plastic and polymer synthesis. These chemicals are conventionally synthesized via toxic phosgene-based technology. Replacement of The current phosgene-based technology by a



R = CH_2Cl, CH_3

Scheme - 1

CO_2-based technology is highly desirable due to its eco-friendliness. Most of the known catalyst systems for the CO_2 based synthesis are homogeneous. They are less stable toward air and moisture or require high temperatures and pressures. Four types of highly efficient, solid catalyst systems are developed for cyclic carbonate synthesis utilizing CO_2. They are i) Zn-W-based polyoxometallates, ii) zeolite-encapsulated metal complexes, iii) titanosilicate molecular sieves and iv) organo-modified mesoporous Ti-SBA-15 materials. With the first three catalysts a homogeneous Lewis base co-catalyst is required for high carbonate yields. With the fourth catalyst system (organo-modified mesoporous Ti-SBA-15) the reaction could be conducted without any additional Lewis base co-catalyst. Further, the reaction could be performed at mild reaction conditions (60 100 psig; 100 - 140°C). The solid catalysts could be reused without any loss in activity/ selectivity (carbamate yield 90%).

The catalysts were found to be highly active for the phosgene-free synthesis of carbamates from CO_2, primary amine and alkyl halide (scheme 2). Carbamate could be synthesized in high yields at mild reaction conditions. Using the above-mentioned solid catalysts the reaction could be conducted in solvent-free conditions.

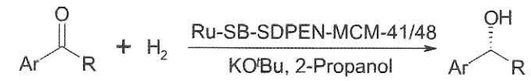
$$2\ R'NH_2 + CO_2 \rightleftharpoons [R'NHCOO^-][R'NH_3^+]$$

$$[R'NHCOO^-][R'NH_3^+] + RX \longrightarrow R'NHCOOR + R'NH_2 + HX$$

Scheme 2

2.1.2.2.5 Heterogeneous asymmetric catalysis

A rational approach towards the synthesis of an efficient heterogeneous catalyst for enantioselective hydrogenation of prochiral ketones, involving anchoring of Ru-(*S*)-BINAP (2,2'-bis(diphenylphosphino)-1,1'-binaphthyl)-(*S*,*S*)-DPEN (1,2 diphenyl ethylene diamine) complex on the inner surfaces of mesoporous MCM-41 and MCM-48 molecular sieves has been developed. This catalyst shows promising activity and excellent enantioselectivity (93-98 % ee) in the hydrogenation of prochiral aromatic ketones, and can be reused several times without any loss in activity and enantioselectivity as shown in table.



Catalyst = 100 mg, Ru; substrate: base = 1: 1400: 20; temp. = 100 °C; H_2 pressure = 1.38 MPa; stirring speed = 400 rpm; duration = 6 h.

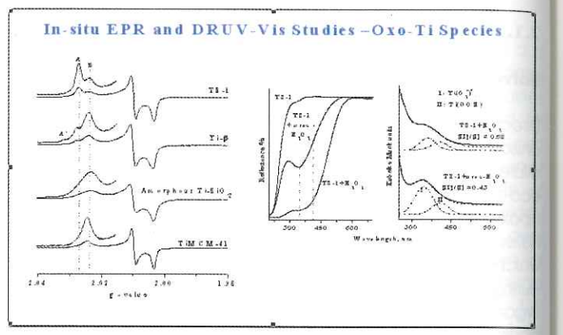
Recycle studies of the heterogeneous catalysts for hydrogenation of acetophenone

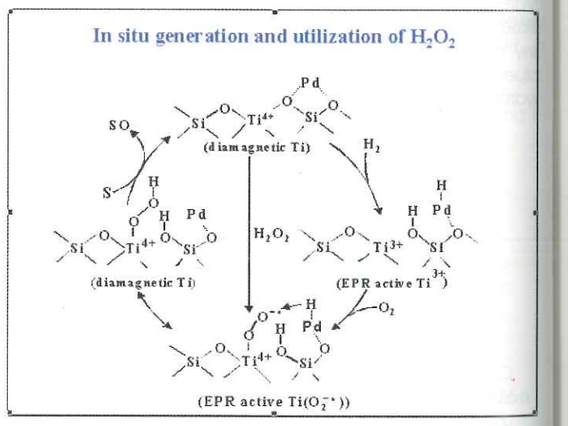
No. of recycles	Ru-SB-SDPEN-SiO_2 conv. (mol %)	ee (%)	Ru-SB-SDPEN-MCM-48 conv. (mol %)	ee (%)	Ru-SB-SDPEN-MCM-41 conv. (mol %)	ee (%)
0	92.0	94	94.0	93	96.0	95
1	78.3.	84	93.7	93	95.9	95
2	58.9	72	93.8	93	95.7	95
3	42.9	71	93.5	93	95.8	95
4	20.6	70	93.3	93	95.4	95

2.1.2.3 In-situ structural characterization of solid catalysts

2.1.2.3.1 Active Ti sites in titanosilicates: EPR and UV-Visible spectroscopy

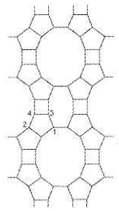
Titanosilicate molecular sieves have been widely investigated for their remarkable catalytic activity in the selective oxidation of a variety of hydrocarbons at mild conditions using H_2O_2 oxidant. In spite of two decades of significant progress there are still many unresolved issues and challenges in this field. The knowledge of the identity and structure of the active sites on titanosilicates, the configuration of the reaction intermediates formed by their interaction with oxidant/ reductant molecules, and the reaction mechanism is not adequately understood. A detailed understanding of this problem might lead to the development of efficient large pore titanosilicate molecular sieves more active than the medium pore TS-1 in the selective oxidation of large molecules of interest to the fine-chemicals industry. With this aim different types of titanosilicates were investigated during reaction conditions using *in situ* EPR, UV-visible and magnetic susceptibility techniques. The interaction of aqueous H_2O_2 and anhydrous urea-H_2O_2 and H_2 + O_2 with titanosilicates revealed for the first time the presence of different types of framework Ti-sites (A and B; see EPR figure). Different types of oxo-Ti species (I: Ti-superoxo and II: Ti-peroxo; see UV figure) were realized. It was found that there exists a correlation between the concentration of different Ti sites/oxo-Ti species and catalytic activity/ selectivity in hydroxylation and epoxidation reactions. This *in situ* spectroscopic method provided deeper insight into the structure of the active sites and their catalytic role. Pd-loaded TS-1 catalyst for epoxidation of small molecules like allyl alcohol and allyl chloride using H_2 + O_2 oxidant is a very recent development. This approach has great potential for an entirely new process for propylene oxide and epichlorohydrin.



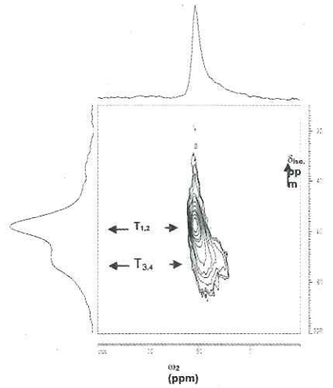


2.1.2.3.2 Bronsted acid sites in mordenite: Multinuclear MAS NMR

^{1}H-^{27}Al REAPDOR Rotational Echo Adiabatic Passage DOuble Resonance (REAPDOR) NMR experiments distinguish structurally dissimilar Brönsted acid sites located in main 12 ring and 8 ring channels of the zeolite mordenite.



Structure of mordenite, shape selective catalyst, used industrially, showing 4 non-equivalent T-sites located in main-12 ring channels and 8-ring side pockets



^{27}Al 3Q-MAS spectrum of NH_4^+/H^+-MOR. The anisotropic projection onto the d_2 axis (top) corresponds to the classical MAS spectrum and displays only a broad tetrahedral resonance. On the contrary, the isotropic projection onto the d_{ISO} axis (left) shows two different tetrahedral resonances labeled as Al^{IV}(I) and Al^{IV}(II) and correspond to the Brönsted acid sites Si-O(H^+)-Al^- and Si-O(NH_4^+)-Al^-, respectively.

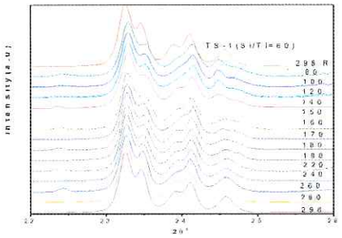
It was observed that the non-equivalent tetrahedral Al sites at the Brønsted acid environments could distinguished by ^{27}Al-[1H] REAPDOR due to the large difference in the dipolar dephasing behavior when proton localization has been achieved. Additionally, evidence from an independent ^{27}Al triple quantum MAS experiment on NH^{4+}/H^+-MOR is presented as shown in figure. Two tetrahedral ^{27}Al resonances [AlIV(I), AlIV (II)] are clearly resolved along the isotropic dimension (dISO) of the 3Q-MAS sheared spectrum. No clue about the multiplicity of tetrahedral Al sites is provided in the ^{27}Al MAS spectrum.

2.1.2.3.3 Mechanistic study on selective N-monomethylation of aniline: FT-IR spectroscopy

Selective N-monomethylation of aniline has been carried out on Cu-Zn ferrospinels and its mechanistic reaction pathway has been explored by *in situ* FT-IR spectroscopy. In a very similar way, phenol methylation to o-cresol and 2,6-xylenol on Cu-Co ferrospinel has been carried out. Partial oxidation of alcohols to value added products like aldehydes and acids has been initiated.

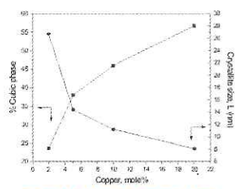
2.1.2.3.4 Structural transitions in titanosilicates and oxide catalysts: non-ambient powder XRD

The location of metal ions in the framework of titanosilicates (e.g. TS-1) and the site occupancies can be identified using variable temperature XRD technique. The structural modifications on cooling high Ti loaded silicalite-1 (Si/Ti=33) samples from room temperature (RT) to 80 K under anhydrous conditions using high resolution powder X-ray diffraction technique and CuK radiation have shown that the phase transition from orthorhombic to monoclinic occurs in the range 165 to 190 K with different Ti concentration. An attempt has been made to locate the probable occupation sites of ti in the framework using the Rietveld refinement technique. Ti occupied the T sites T2, T3, T4 and T5 and it appears that the T4 site is preferentially occupied as compared to others and these contribute to the formation of peroxo, hydroperoxo or superoxo radical enabling facile oxygen transfer to the substrate. The location of the acid sites in the channels and cavities control its catalytic application. Further studies with different metallosilicates are in progress.

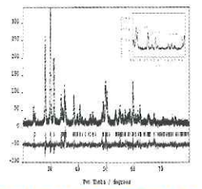


Multiple plot of LTXRD patterns of a typical TS-1 sample

Zirconia-based solid catalysts are finding increasing applications in H_2 generation, 3-way catalysis, low temperature CO oxidation, etc. The structure of zirconia has a marked effect on the metal dispersion. *In situ* high temperature XRD (HTXRD) studies on these materials would be highly useful to examine the structural changes of the support and its consequences on metal dispersion at reaction conditions. The discrepancies in the reports on zirconia and the inconsistencies in the literature are mainly with reference to the structural properties of zirconia, which alter as a function of temperature or doping of other metal atoms in the lattice. Rietveld refinement studies carried out on the RT and HTXRD profiles of copper stabilized zirconia samples revealed that zirconia has not been stabilized into the cubic phase alone and is a mixture of cubic and tetragonal



Crystallite size and the relative % with copper content



Rietveld refinement of $Zr_{1-0.8}Cu_{0.2}O_{2-}$ scanned at 1173 K

phases. There is an increase in the concentration of cubic phase at the expense of tetragonal phase with increase in temperature and with a steady increase in crystallite size. Higher concentration of dopant copper and smaller crystallite size are the governing factors in the stabilization of zirconia into cubic phase.

2.1.2.3.5 Mechanistic investigations using molecular beam experiments

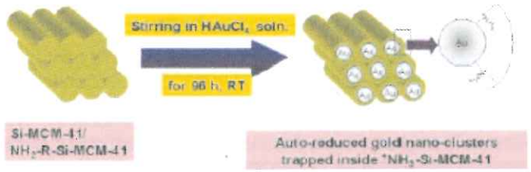
Fundamental studies on NO dissociation reactions have been carried out without any reductant and with CO as reductant on Pd(111) surfaces in a molecular beam equipment. First time NO dissociation could be seen on Pd(111) surface at high flux

conditions indicates the catalytic activity. Systematic studies indicate the changes in sticking coefficient and other basic factors. NO+CO reaction is active in the temperature window of 425-625 K. CO displacement by NO was observed clearly in the reaction indicates the stoichiometry of reactants on the surface is considerably different from the reactants mixture composition and influences the reaction. CO oxidation studies also have been carried out and indicate the bistability of the reaction on Pd(111) surfaces at certain conditions and hints the initial state of the catalyst surface very strongly influences the reaction rate.

2.1.2.4 Nanotechnology in catalysis

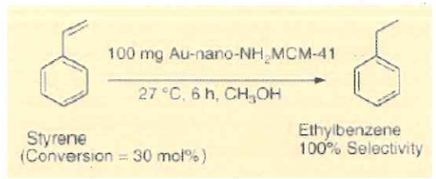
2.1.2.4.1 Formation and entrapment of gold nanoparticles in organo-functionalized mesoporous silicas

A novel method for simultaneous formation and entrapment of gold nanoparticles in NH_2-propyl-Si-MCM-41 was developed. From the results it could be concluded that gold nanoparticles can be conveniently synthesized and stabilized in siliceous matrices, ordered or amorphous. The silanol groups present on the surface of host matrices participate in the reduction of aqueous chloroaurate ions to form the nanoparticles. When amorphous silica was used as the host, size of the nanoparticles could be controlled by external addition of alkylamine molecules. The alkylamine molecules form self-assembled monolayers on the surface of the gold nanoparticles during the initial nucleation period, and thus prevent further growth. Particle size is dependent on concentration and alkyl chain length of the alkylamine molecules. However, when organo-functionalized MCM-41 was used as the host, the addition of alkylamine molecules was not at all necessary. The presence of pendant NH_2 or SH functional groups inside the mesopores, evidenced from solid-state NMR experiments, serve the same purpose by entrapping the gold nanoparticles through covalent interactions just after their formation.



The probable structure of the NH_2-MCM-41 material before and after immersion in $HAuCl_4$ solution for 96h. The magnified view of the cross-section shows the entrapped gold nanoparticles formed by spontaneous reduction of chloroaurate ions by the MCM-41 material

It was further demonstrated that the gold nanoparticles supported on organo-functionalized MCM-41 materials exhibit good catalytic activity in the hydrogenation of unsaturated olefinic substrates. In fact, these materials show better catalytic activity than the fumed silicagold nanocomposites, obviously due to smaller particle sizes. This makes the nano-Au-MCM-41 materials budding systems for future applications in catalysis as shown in scheme.



Conversion of 1-hexene on different supported gold catalysts

Catalysts	Mean diameter of Au	Conversion of
Au-BH-SH-MCM-41°	nanoparticles (nm)	1-hexene (mol. %)
nano-Au-NH_2-MCM-41	3.5 0.7	18.1
nano-Au-SH-MCM-41	3.4 0.5	18.5
SiAu5	3.2 0.5	18.7
SiAu400	17.2 0.5	6.8
SiAuDDA1	20.6 0.5	7.2
SiAuDDA3	10.0 0.5	8.7
SiAuDDA6	15.9 0.5	7.6
SiAuNOA3	18.8 0.5	9.6
SiAuODA3	21.3 0.5	5.1
	10.5 0.5	8.3

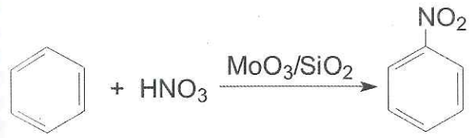
Reaction conditions: temperature = 150 °C; H_2 pressure = 5.5 MPa; duration = 8 h.°-Au nanoparticle formed from borohydride reduction of aqueous $HAuCl_4$

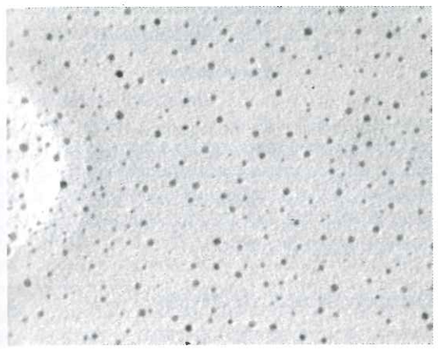
2.1.2.4.2 Silica supported MoO_3 nanoparticles for nitration of aromatics

Nitration of aromatic substrates is a widely studied reaction because of its industrial importance as many nitro aromatics are extensively used as intermediates for the manufacture of dyes, pharmaceuticals, perfumeries and pesticides. Conventionally nitration of aromatics is carried out using a mixture of nitric and sulfuric acids. The waste generated during the course of the reaction contains dilute sulfuric acid and its disposal and recycle is a major problem. The nitration of benzene, chlorobenzene, toluene, xylenes, phenol, fluorotoluenes, naphthalene, etc has been carried out using various solid acid catalysts. The use of solid acid catalyst not only eliminates the use of sulfuric acid but also ensures good selectivity for the desired products.

A catalyst, which is mesoporous silica supported MoO_3 nanoparticles using modified sol-gel process has been synthesized. It showed a very high activity for vapor phase nitration of benzene at lower temperature. Benzene was nitrated using concentrated nitric acid (70 %) in liquid phase over solid acid catalyst (new solid super acid). The results indicate 100 % selectivity for nitrobenzene and maximum conversion of nitric acid (90-95 %) with no deactivation of catalyst.

A laboratory scale process has been developed using this catalyst, which showed good potential for the commercialization. The product nitrobenzene has been analyzed and meets the specifications. An industrial customer has shown interest in the process and a plan is being worked out to set up the plant to scale-up the laboratory process in customer's premises.



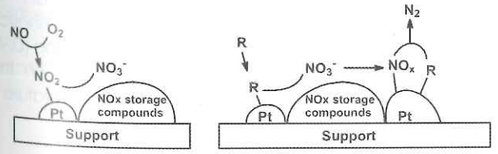


TEM of MoO_3 /SiO_2 catalyst

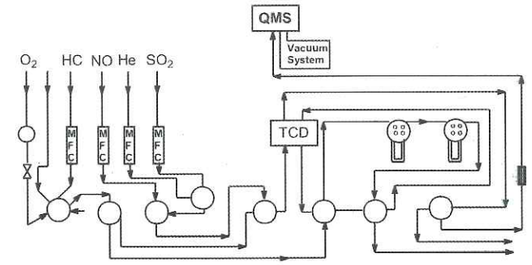
2.1.2.5 Environmental clean-up

2.1.2.5.1 DeNOx catalyst for lean-burn diesel engine

Diesel engines are popular because of their fuel efficiency compared to gasoline engines as they operate under very lean conditions (excess of oxygen as compared to the stoichiometric A/F ratio) and operate with high compression ratio. The conventional three-way autoexhaust catalyst is not active for NOx reduction due to the presence of excess oxygen in the diesel engine exhaust. Efforts are being made to find out an efficient catalyst to reduce NOx under lean-burn conditions. Two different approaches are adopted for removal of NOx from diesel engine exhaust. First is direct reduction of NOx using hydrocarbon and second is NOx storage reduction (NSR). The work is being done on the second approach, i.e., NSR. In this approach NOx is stored on the catalyst as nitrate under lean conditions. When catalyst is saturated with nitrate, a pulse of hydrocarbon is given to reduce nitrate to N_2 and hydrocarbon gets oxidized to CO_2. The necessary reactor facility has been set-up for the evaluation of the catalytic activity for NOx removal. Few catalysts have been synthesized with various compositions and using different synthetic techniques. These catalysts have been characterized using various characterization techniques and NOx storage behaviour has been studied using *in situ* IR studies. The catalytic activity for deNOx storage and reduction has been evaluated using online mass spectrometer and the results are encouraging.



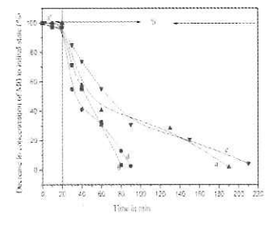
R = Reducing agent



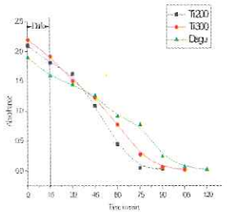
Schematics of the reactor fabricated

2.1.2.5.2 Photocatalysis using nanocrystalline titania

Nanocrystalline titania of different crystallite sizes (2-18 nm) have been made without any impurity of brookite or rutile using a novel ultrasonication technique which have shown higher photocatalytic activity for the decomposition of monochlorobenzene and methylene blue dye in the UV region. The modified nanocrystalline samples using hydrogen peroxide are more effective as a photocatalyst in the visible light. These catalysts are found be active in the epoxidation reactions too.



Photocatalytic activity in UV light

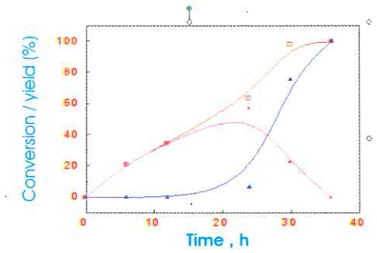


Photocatalytic activity in visible light

2.1.2.6 Biocatalysis and biosynthesis of nanomaterials

2.1.2.6.1 Biocatalyst for selective synthesis of lactones from cyclic ketones

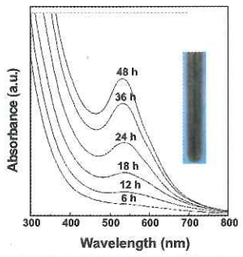
Fusarium oxysporum f. sp. was found to be an efficient and selective biocatalyst for the biotransformation of cyclohexanone and cyclopentanone into ε-caprolactone and δ- valerolactone, respectively, in quantitative yields. The whole cell mycelia of the fungus were used in the absence of any externally added co-factor like NADP or NADPH. Figure depicts the biotransformation of cyclohexanone to cyclohexanol and caprolactone using *Fusarium oxysporum*.



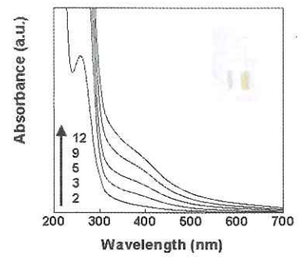
Progress curve of ketone transformation with *F. oxysporum f. sp. ciceri* NCIM 1282, A: cyclohexanone; B: cyclopentanone; curve a (¤) = conversion of ketone, curve b (•) = yield of the corresponding alcohol, curve c (•) = yield of lactone. Reaction conditions: biocatalyst concentration = 20 gm wet wt/ 100 ml reaction medium, temp = 28°C, shaker speed = 200 rpm, substrate concentration = 100 mg / 100 ml reaction medium.

2.1.2.6.2 Biosynthesis of nanomaterials

The development of reliable, eco-friendly processes for the synthesis of nanoscale materials is an important aspect of nanotechnology. As part of our ongoing investigation into the use of fungi for nanoparticle synthesis, depending on the reaction conditions of the fungus *Tricothecium* sp. with aqueous gold ions it was found that gold nanoparticle synthesis can be controlled to occur either within the biomass or extracellularly. More specifically, it has been found that reaction of gold ions with the *Tricothecium* sp fungal biomass under stationary conditions results in the rapid extracellular formation of gold nanoparticles of spherical, rod-like and triangular morphology whereas reaction of the biomass under shaking conditions resulted in intracellular growth of the nanoparticles. It is believed that on changing the reaction conditions of the fungus with gold ions, the concentration of enzymes and proteins which are being released into the medium under stationary and shaking conditions varies resulting in the formation of extracellular/ intracellular gold nanoparticles. The gold nanoparticles are not toxic to the cells and the cells continued to grow after the biosynthesis of the gold nanoparticles in both the cases. Below is an example of biosynthesis of gold nanoparticles CdS nanoparticles using fungus *Tricothecium and Fusarium oxysporum*, respectively.



UV-vis spectra recorded as a function of time of reaction of a 10^{-3} M aqueous solution of $HAuCl_4$ with *Tricothecium* sp. biomass grown in stationary phase. The inset shows a test tube of the gold nanoparticle solution formed at the end of the reaction (48 h).

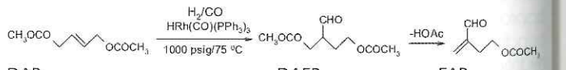


UV-vis spectra recorded from the aqueous 10^{-3} M $CdSO_4$ solution as a function of time of addition of the fungal biomass. The time of reaction (in days) is indicated next to the respective curves. The inset shows test-tubes containing the $CdSO_4$ solution before (test-tube on the left) and after reaction with the fungal biomass for 12 days (test-tube on the right).

2.2 Homogeneous catalysis

2.2.1 Hydroformylation of 1,4-diacetoxy-butene to vitamin-A intermediate

Hydroformylation of substituted olefins is gaining considerable attention in catalytic synthesis of several complex organic intermediates with applications in fine chemicals, pharmaceuticals and specialty chemicals. The application of hydroformylation in organic synthesis is highly promising as it provides a clean catalytic route with high atom efficiency to substitute the conventional reagent based synthesis. The synthesis of α,β-unsaturated aldehydes by the hydroformylation of 2-alkenyl acetates and subsequent elimination of acetic acid are used for the production of intermediates, which are of interest in terpene chemistry having great significance in perfumery applications. Another important example of this class is the hydroformylation of 1,4-diacetoxy-2-butene (DAB) to obtain 1,4-diacetoxy-2-formyl butane (DAFB), which is an intermediate in synthesis of Vitamin-A acetate. Reaction is as shown below:



DAB DAFB FAB

The objectives of this project are: i) development improved catalyst for catalyst/ product separation. Rhodium catalyst for hydroformylation of DAB, ii) investigation of kinetics in detail, and iii) development of heterogenized catalyst for catalyst/ product separation.

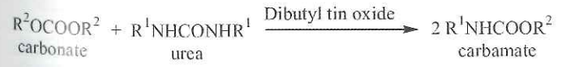
Hydroformylation of 1,4-diacetoxybutene using homogeneous $HRh(CO)(PPh_3)_3$ catalyst was investigated with the aim to understand product distribution, selectivity and intrinsic kinetics. The effect of $HRh(CO)(PPh_3)_3$ and 1,4-diacetoxy 2-butene (DAB) concentrations, and CO and H_2 partial pressures on the concentration vs. time profiles was studied over a temperature range of 338 to 358 K. A detailed analysis of the kinetic models was carried out using the integral batch reactor data for the homogeneous catalyst to develop rate equations for both the hydroformylation and deacetoxylation steps. The activation energies were found to be 75.24 and 108.9, kJ/mol respectively. Heterogenized catalysts also have been prepared by encapsulation and tethering techniques. For the first time, it has been shown that hydroformylation as well as deacetoxylation takes in single step (tandem synthesis) to give FAB with 100% selectivity. Catalyst is active and selective even after 5 recycle experiments.

2.2.2 Carbamate synthesis

Carbamates are useful compounds having wide range of applications in chemical industry such as in the production of commodity chemicals like polyurethane, herbicides and pesticides. On the other hand carbamates are required in low volumes but high cost category segment in specialty chemical industry for the production of drug intermediates in pharmaceutical industry. They are also used in the production of highly value added drug intermediates in pharmaceutical industry. In organic synthesis carbamates are often used as protecting groups for amine functionality. The conventional process for the carbamate synthesis is based on phosgene technology; this process besides being highly energy intensive uses highly corrosive phosgene and produces hydrochloric acid as a side product. Efforts are continuously being made for the replacement of phosgene-based technology with environmentally benign routes such as carbonylation of nitro compounds, oxidative carbonylation of amines, carboxylation of amines using organic carbonates or carbon dioxide and alcoholysis of urea.

The objective of this work is to develop an improved method for carbamate synthesis using organo-tin catalyst wherein applicability of our protocol is extended to synthesize wider range of carbamates by reacting ureas and carbonates.

The route developed is based on two industrially important methods for the synthesis of carbamates viz., alcoholysis of ureas and carboxylation of amines. Synthesis of carbamate derivative from urea and carbonate using various homogeneous catalyst has been carried out and it was found that tin complex catalysts such as DBTO shows excellent activity and selectivity. The effect of reaction parameters such as temperature, concentration of reactants, catalyst, effect of solvent etc. were examined. In a typical optimized conditions 93 % yield of N-phenyl phenyl carbamate have been realized at 150 °C in 4h reaction time.



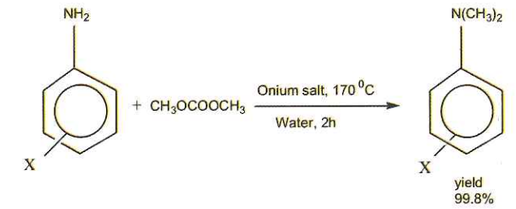
2.2.3 N-alkylation of amines to dimethyl aniline

N,N-Dimethyl anilines (NNDMA) are useful intermediates in the synthesis of dyestuffs, pharmaceuticals and agrochemicals as well as fine chemicals such as vanillin, michler's ketone etc. They are also used as solvents and additives in the production of synthetic rubber. N,N,N',N' -Teramethyl-1,4-phenylene diamine is used in the bio-medical field as a reagent known as Wurster's blue.

Conventional alkylating agents are not good from environmental point of view e.g. alcohols as alkylating agents are effective only at higher temperatures (>250 °C) besides the formation of side products such as toluidines due to ring alkylation. The results on N-alkylation of anilines with organic carbonates indicate that, while mono alkylated products are formed selectively in the liquid phase alkylation, dialkylated products are difficult to synthesize selectively. Therefore, it is most desirable to produce selectively NNDMA in high yield.

The objective of this work is to develop an environmentally benign catalytic route to synthesize selectively N,N-disubstituted alkyl anilines in high yields and almost free from side products such as mono alkylated anilines, carbamates and alkyl toluidines using DMC as methylating agent and onium salts as catalysts.

Selective synthesis of dialkylated product by N-alkylation of aromatic amines using dimethyl carbonate requires high temperatures in the range of 250-300 °C.



At comparatively low temperatures (< 200 °C) monoalkylated amine and carbamates are formed as side products. In the present investigation it was shown that onium salt as catalyst in presence of small quantities of water selectively gives dimethyl aniline in 99.8% yield at 170 °C in two hours.

2.2.4 Single step process for the preparation of p-aminophenol via catalytic hydrogenation of nitrobenzene

p-Aminophenol (PAP) is an intermediate for making paracetamol, a widely used antipyretic and analgesic drug. Conventional method of preparation of p-aminophenol involves Fe/HCl reduction of p-nitrophenol, which poses a serious effluent problem, due to generation of large amount (1.2 kg/kg product) of Fe-FeO sludge. Development of a catalytic single step process for p-aminophenol via hydrogenation of nitrobenzene was undertaken.

the process optimization work is in progress and the PAP selectivity has been enhanced from 58 to 70% by pretreatment of the catalyst and modifying the work up procedure. A successful bench scale demonstration was given (2 liter and 300 ml scales) to the sponsor. Based on the bench scale process, a basic engineering package (BEP) for pilot plant (100 liter vol. reactor) has been prepared and given to the industrial customer.

2.2.5 Development of process for 4-hydroxybenzaldehyde

Catalytic liquid phase oxidation of substituted toluenes by air/oxygen to the corresponding aldehydes is of great industrial importance. One such example is p-cresol oxidation to 4-hydroxybenzaldehyde(PHB) which is a starting material for the manufacture of vanillin. PHB is also used as an additive for metal plating brighteners, in perfumes and in liquid crystals. Conventionally, PHB is obtained as a by-product from Reimer-Tiemann reaction of salicylaldehyde with phenol. Work on catalytic liquid phase oxidation of p-cresol to PHB with an objective to develop a catalyst and a bench scale process for PHB has been started.

A cobalt based catalyst which can give > 93% selectivity to PHB with complete conversion of p-cresol has been developed. The reaction conditions like temperature, p-cresol concentration, catalyst loading, and oxygen partial pressure have been optimized to give the highest conversion and selectivity to PHB. Collection of other relevant data for determining the kinetics of this reaction is in progress.

2.2.6 Studies in multiphase reactors

Modeling of a bubble column slurry reactor

A bubble column slurry reactor model has been developed for the hydrogenation of aqueous maleic acid (MAC) to tetrahydrofuran (THF). This particular reaction system has recent commercial relevance and represents a case where complex multi-step catalytic hydrogenation reactions are conducted at high pressure (>15 MPa) and high temperature (>240° C). It also has additional complexities associated with the reaction chemistry since the THF reaction product is volatile and the reaction is highly exothermic. The model proposed here is derived using the mixing cell approach and incorporates the contributions of gas-liquid and liquid-solid mass transfer, intraparticle diffusion effects, product volatility, heat effects and complex multi-step reaction kinetics. The effect of gas and liquid velocities, catalyst loading, inlet maleic acid concentration, and temperature on the conversion, selectivity, temperature rise and productivity of the desired products (THF and γ-butyrolactone (GBL)) is also discussed. Since the reaction step involving the hydrogenation of GBL to THF is relatively slow, severe operating conditions are necessary to achieve high THF selectivity. The distribution pattern of THF in the gas and liquid phases is also discussed. The model proposed could be useful for simulation of existing pilot or industrial scale reactors as well as the design and scale up of new reactors for this particular reaction or one that has similar characteristics.

Esterification using ion exchange resin catalysts

The ion exchange catalysed esterification of the reactions systems, i) kinetics of esterification of acetic acid with methanol using Dowex 50W catalyst, ii) kinetics of esterification of acetic acid with butanol using Dowex 50W catalyst and iii) kinetics of esterification of maleic acid with methanol using Dowex 50W catalyst have been studied. While the first two processes are used as case study of esterification reaction to account the homogeneous reaction in simultaneous homogeneous-heterogeneous catalytic reaction, the third problem is challenging as it involves esterification of dibasic acid, which have commercial value.

For all the systems under consideration, kinetic equations have been developed using extensive experimental data obtained over a wide range of operating conditions. In evaluating the kinetics the contribution of both homogeneous and heterogeneous reactions have been taken into account. Batch and fixed bed reactor models have also been developed, and the model predictions compared with experimental data.

2.2.7 Racemization of 2-aminobutanol to dl 2-aminobutanol

Ethambutol hydrochloride (N,N'-ethylene bis (2-aminobutanol) di hydrochloride) is one of the drugs used in combination with other anti-tubercular drugs and it helps to boost their effects. Optical resolution of *dl* 2-amino -1-butanol gives *d* 2-amino -1-butanol, which is used in the manufacture ethambutol hydrochloride. The undesired isomer *l* 2-amino 1-butanol has no utility. It is highly desirable to convert this undesired isomer into racemic mixture so that it can be again resolved to get *d* isomer. The aim of this project is to develop an optimum process for racemization of *l* 2-aminobutanol to *dl* 2-aminobutanol and carry out the catalyst recycle studies.

The preliminary investigation on racemization, identification of by-products formed and optimization of the reaction parameters has been done. Effect of various reaction parameters like time, substrate concentration, catalyst concentration, temperature and pressure on extent of racemization and by-product formation has been studied. Study on catalyst recycle is in progress.

2.2.8 Hydrogenation of ethylene glycol

Ethylene glycol of high purity is required for the preparation of polyesters. Recycled ethylene glycol used as a feed for this purpose, contains low levels of organic, metallic and oligomeric impurities. Hydrogenation in the presence of a catalyst can remove organic impurities in the recycled ethylene glycol. The objective is to determine the degree of removal of the impurities present in recycled ethylene glycol by hydrogenation in a continuous trickle bed reactor and to determine the change in catalyst performance over a period of time.

A preliminary investigation in a trickle bed reactor using synthetic feed for catalysts supported on carbon has been completed. The effects of various reaction parameters like catalyst loading, temperature, pressure and liquid flow rate have been studied. The performances of the catalysts have also been evaluated for the recycled ethylene glycol.

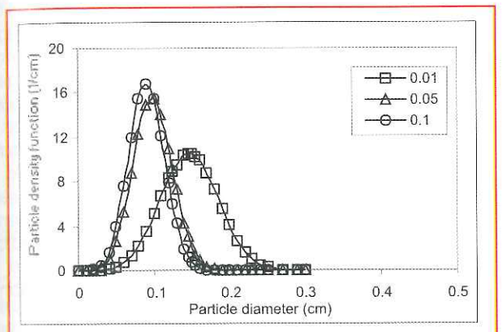
3. Chemical engineering science

3.1 Polymer & catalytic reaction Engineering

3.1.1 Polymer reaction engineering

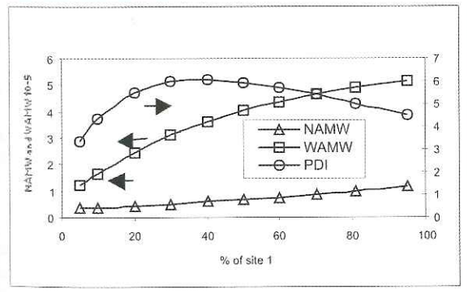
Dynamic model for polypropylene fluidized bed reactor: PORE

Gas phase propylene polymerization process is a complex process wherein small catalyst particles (20 - 80 mm) react with the incoming fluidizing gas (monomer) to form a broad distribution of polymer particles (100 5000 mm).



Effect of catalyst feed rate on PSD

At the same time, final polymer properties can change drastically depending upon the nature of catalyst (active sites, deactivation, transformation rates etc.). A mathematical model capable of predicting the simultaneous effects of complex kinetics and particle size distribution is essential to completely understand and optimize the performance of the system.



Effect of site ratio on NAMW and WAMW

PoRE(*Po*ly-olefin *RE*actor simulator) is a software built around a comprehensive mathematical model to simulate transient behavior of fluidized bed polypropylene reactors. Rigorous polymerization kinetics (which include several activation, deactivation, transformation, chain transfer and propagation reactions) applicable for multi-site catalyst with more than one monomer is incorporated in the model. Particle size distribution is predicted by solving steady-state population balance equations after steady state is achieved. The model is capable of predicting the effects of operating conditions such as superficial gas velocity, temperature, pressure and catalyst feed rate on polymer properties and PSD of the product stream.

3.1.2 Catalytic reaction engineering

Modelling of FCC riser reactors

Fluid dynamics of a FCC riser reactor is extremely complex. Computational fluid dynamics based modelling offer powerful tools to understand such complex fluid dynamics and to realize the desired solid and temperature profiles within the riser reactor. Coupled with reaction engineering models, such CFD models offer unique tools to enhance performance of FCC systems. Such models are being developed under this project. Three layers of computational models namely, i) mixing and evaporation of oil droplets with hot solids, ii) gas-solid flow in riser reactor, and iii) cracking reactions in riser reactor, are being developed. Process of three-phase mixing with phase change occurring in the bottom region of a riser reactor will be thoroughly analysed. Computational flow models are being developed in three stages, viz., i) fully developed gas-solid flow, ii) extension to developing flow, and iii) extension to three-phase flow with evaporation. Emphasis will be given on developing predictive models to simulate influence of particle characteristics, solids flux, gas velocity and riser diameter. The developed models will be mapped on to commercial CFD code, FLUENT (of Fluent Inc., USA). The CFD model will communicate with riser reactor model in real time. Riser reactor model based on mixing cell framework will be developed to simulate cracking reactions. The models will be validated by comparing predictions with published information and data from Indian refineries, if available. The model will be able to predict the dynamic behaviour of riser reactor and will be useful for performance enhancement.

3.2 Flow modelling

3.2.1 Modeling of multiphase flows

A comprehensive study of fluid dynamics of gas-liquid reactors (stirred and bubble column and trickle beds) has been initiated. New ways of characterizing inherently unsteady flow in these gas-liquid reactors are being developed. Arrays of pressure and voidage probes (to measure wall pressure and gas hold-up fluctuations) will be used to capture and to study the dynamics of gas-liquid flows. Possible ways of reducing the complex dynamics to fewer degrees of freedom based on phenomenological models will be explored. Rigorous computational fluid dynamics based models have been developed to guide the phenomenological modelling. Eulerian-Eulerian and Eulerian-Lagrangian models were developed to simulate gas-liquid flow in bubble columns. These CFD models were verified and validated by comparing predicted results with experimental data. The modelling framework and understanding gained during the project will be

used to develop robust and powerful tool (like stethoscopes) to characterize, to control and to optimize the fluid dynamics of dispersed multiphase reactors.

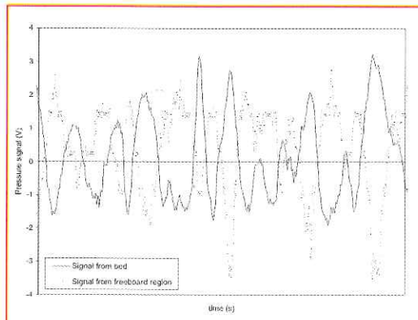
3.2.2 Modeling of membrane spacers

Detailed CFD models are developed to simulate complex fluid dynamics of membrane modules. CFD models were used to enhance existing understanding fluid dynamics of membrane modules and to study influence of spacer shapes and configuration on the fluid dynamics. The emphasis is on understanding influence of curvature of spiral membrane modules on fluid dynamics. The computational experiments will be carried out to identify optimum shape of spacers for different conditions and to develop strategies for performance enhancement.

3.2.3 Modeling of filament interaction

Drag coefficient on a yarn in a spinning cell together with mass and heat transfer coefficients are important parameters affecting both the drying of thread lines and the formation of yarn properties. Computational study of axial flow over single- and multi-filament thread lines was therefore undertaken. Certain simplifications regarding the diameter variation and properties of the fibers were invoked. Analytical solutions were obtained for certain limiting cases. Computational fluid dynamics (CFD) based models were developed to simulate flow, drag and other transport processes from the moving fiber(s) with an axial flow of gas. Computational model was verified by comparing with analytical solutions. Simulations will be carried out at various parameters covering the relevant range of interest (fiber velocities, diameters, gas flow, number and spacing of filaments). The simulated values of drag, heat and mass transfer coefficients will be presented in the form of correlations. These results will enhance the accuracy and the reliability of the simulations of spinning chambers.

3.2.4 Characterization of polypropylene fluidization

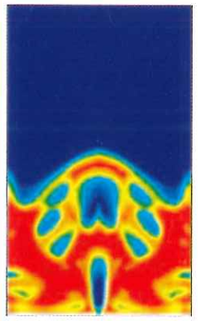


Pressure fluctuations recorded inside the bed and in the freeboard region

Fluidized bed solid catalyzed propylene polymerization is one of the main and important routes to produce polypropylene. The fluidization behavior of polypropylene particles is critical in designing the reactor. If the gas phase is not equally distributed throughout emulsion phase then, in some parts of the reactor, there is a danger of excessive heating of polymeric particles to the point of melting and forming large polymer chunks. On the other hand, lack of monomer in the vicinity of a growing polymer particle may yield sub-optimal polymer properties. Further, the fluidization behavior of polypropylene is complicated because of wide particle size distribution and agglomeration of particles. Therefore, understanding the fluidization behavior is vital in successfully designing and scaling up the polypropylene reactor.

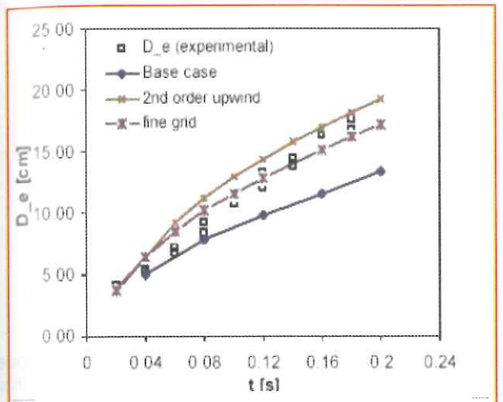
The fluidization behavior of polypropylene resin was studied using analysis of wall pressure fluctuations. It was observed that the signals obtained from the bed region and freeboard region are in 180° phase shift indicating bed surface phenomena to be one of the root causes of fluctuations. The change in fluidization state could be identified by the analysis of power spectra and dominant frequency. Nonlinear dynamic tools like Kolmogorov entropy were used to provide quantitative information about the fluidization; efficient ways should be employed to extract maximum information from a time series using these tools. Wall pressure fluctuations measurement is found to be a useful tool to characterize the flow in fluidized bed reactors. More experimentation is needed in order to completely understand the effect of particle size distribution on polypropylene fluidization.

3.2.5 Bubble formation at single orifice



Typical voidage profile

Many unique properties of fluidized beds can be attributed directly to the presence of bubbles and fluid dynamics of fluidized beds is dominated by bubble behavior. Therefore, accurate prediction of bubble characteristics such as the size distribution, the bubble rise velocity distribution and the bubble frequency distribution is very important. However, these distributions depend on the initial bubble characteristics at the gas distributor, where the bubbles are generated. Furthermore, the gas-solids contacting efficiency of fluidized bed reactors is quite sensitive to the bed hydrodynamics just above the gas distributor plate. Mass and heat transfer processes are seriously affected by the mechanism of bubble formation. Thus accurately predicting formation of bubbles at the orifice is of extreme importance.



Experimental and predicted bubble sizes

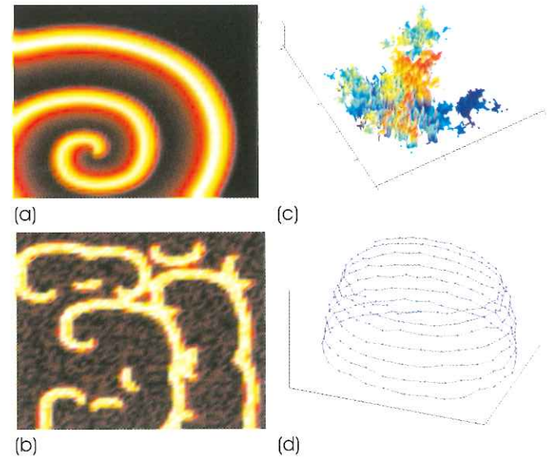
This project is aimed at developing a dynamic Eulerian-Eulerian CFD model for bubble formation at a single orifice. The model is based on two fluid theory, which assumes both the gas and the solid phases as continuum phases. Model simulations were carried out using FLUENT 6.1.18 (of Fluent. Inc.). Preliminary numerical experiments were performed to resolve the issues of grid size, discretization scheme etc. on bubble formation. Numerical experiments were then performed to assess the effect of various parameters such as drag, granular viscosity, frictional viscosity etc. on the bubble formation process. The simulated results obtained from this model were compared with the results obtained from approximate bubble formation models.The computational model and presented results will provide a better understanding of the bubble formation process in fluidized bed reactors.

3.3 Modelling simulation and control

3.3.1 Phenomenology

Isometric graphing and multidimensional scaling (IGMDS) formalism for modelling complex systems and space-time pattern recognition

A fresh approach for studying systems exhibiting complex space-time dynamics and patterns from data has been developed. This new approach, acronymed (igmds), effectively uses isometric graphing and multidimensional scaling formalisms along with geodesic distance definitions to identify and analyze complex networks. For example, the methodology when applied to a reacting system gives considerable insight into clustering properties of reactions taking place on different types of surfaces (ranging from the crystalline to the amorphous and fractal). Pattern recognition by igmds is efficient because high dimensional snapshot data may be studied with increased accuracy and in significantly reduced dimensions when compared with conventional principal component analysis (PCA) algorithms and its analogs. Results obtained with interesting cases of spiral pattern formation and even turbulence on surfaces show that effects of fractality could become very relevant in system performance. With advances in experimental techniques (e.g., atomic force microscopy (AFM) for imaging surface dynamics, LEEM, monitoring velocities as a function of time and space in 3D, etc.), IGMDS shows considerable potential for real-life applications.



IGMDS formalism for studying pattern formation and their recognition in reacting systems. (a) Spiral reaction patterns formed on crystalline surface; (b) Break-up of spirals into turbulence; (c) Example of a fractal amorphous surface; and (d) Data analysis using low-dimensional IGMDS coordinates facilitate space-time pattern recognition and characterization in complex systems (e.g., shown here for the spiral space-time dynamics)

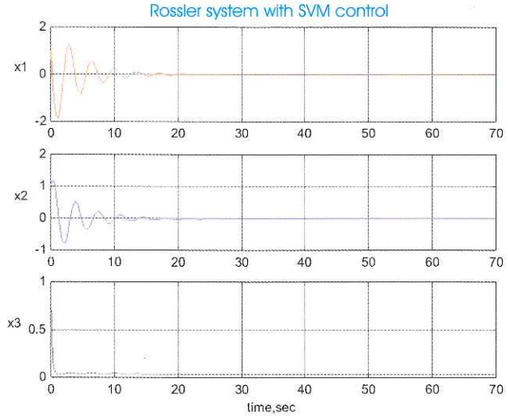
3.3.2 Process modeling

Support vector machines

Support Vector Machine (SVM) classifiers are a set of universal feed-forward network based classification algorithms based on the statistical learning theory and structural risk minimization principle. For classification problems, which are employed in process fault detection and process identification and control, SVMs minimize training and generalization errors simultaneously by minimizing the norm of the feature weights, i.e. by controlling the size of the feature weights. In addition, SVMs map the input vectors into a very high dimensional nonlinear feature space and construct a hyperplane, which linearly separates the data into different classes. This hyperplane is called the maximal margin hyperplane because it maximizes the distance between the closest points of the two classes. Working with a high dimensional feature space introduces the curse of dimensionality. SVMs tackle this problem by appropriately defining a kernel function relating the data in the input space,

to the dot product between the data vectors in the feature space. A robust fault detection SVM methodology has been proposed and successfully applied it to detect conditions leading to faulty yarn quality in rayon manufacturing and to identify different cultivars of wine from its chemical composition. Hybrid Genetic-Quasi-Newton approach for tuning the algorithm parameters was proposed to make the algorithm error free and robust. Additionally, we have proposed "Data Symbolization" has been proposed to deal with unwanted features in the data such as noise and extraneous features. This particular methodology gave good results in presence of noise on many benchmark classification problems (wine classification, bacterial growth/no growth classification etc.).

Rossler system with SVM control

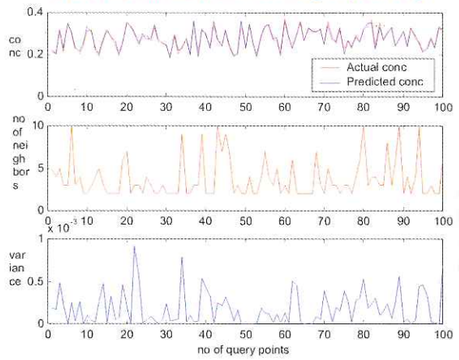


SVM is applied to solve regression kind of problems. In one such application, it is used in controlling the complex nonlinear systems by compensating for the nonlinear part. Once the non-linearity is identified with SVMs, simple linear feedback control law is applied to control the system. The methodology was tested on two important chaotic oscillators (viz. Rössler and Lorenz) and found to be showing excellent performance.

Lazy learning

The input/output mapping [y = f (x)] of a highly nonlinear process may exhibit reasonably smooth behavior over a certain domain of variables and may possess very uneven or peaky surfaces for certain other domain of variables. The global models try to obtain a relationship that approximates the actual mapping with least overall error over the entire domain of variables. It is possible that the model is very accurate in certain regions and not so much in certain other regions. In other words, the single global model may have different extents of error in different regions of the variables span. It is more advantageous in such cases to build local models. ***Lazy learning*** is one such recently introduced nonparametric regression technique that employs a memory based local learning approach. Employment of (i) local weighted regression for parametric identification and (ii) PRESS statistic to assess a local model for structural identification, are the two unique features of Lazy learning. Being a memory based technique, it does not require separate training, which greatly enhances the speed of implementation.

System identification for CSTR using lazy learning



This is illustrated by solving three important problems in process engineering comprising boiling point prediction of aliphatic hydrocarbons using quantitative structural property relations, system identification for a continuous stirred tank reactor in which an exothermal irreversible reaction between sodium thiosulfate and hydrogen peroxide occurs and a fermentation process for polyol production. The performance of the proposed method was found to be very competitive with some of the state-of-the-art approaches.

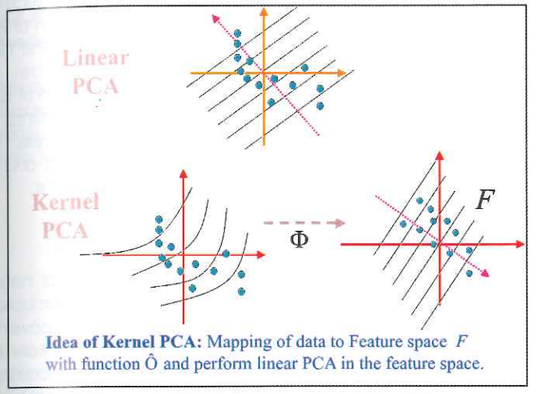
Kernel principal component analysis for data-driven modeling

Principal component analysis (PCA) is a established methodology often used for process monitoring and identification. linear PCA utilizes second order statistics and can extract only the linear features of the data. To capture the correct phase details of the data set and to identify the dominant features existing between variables, a nonlinear version of the PCA should be employed. A Kernel based PCA methodology,has been proposed and elegant nonlinear generalization of the linear PCA for (i) denoising chaotic time series and, (ii) prediction of properties of polymer nanocomposites developed in our laboratory. Use of simple matrix algebra in simulations makes the method an attractive alternative to some hard optimization based methodologies.

On-line monitoring of TCB nitration reaction for abnormality detection in the process

software for process monitoring of TCTNB 1,3,5-trichloro-2,4,6-trinitro benzene plant at HEMRL, Pune using *support vector machines*. has been developed (TCTNB) is manufactured by the nitration of TCB (trichlorobenzene), (TCB) which is very hazardous reaction due to excessive exothermicity, complex nature of reaction mechanism, high reaction temperature, reaction time, etc. So it is very likely that the reaction may undergo abnormality leading to run-away situations. Thus the job of the software developed is to detect the abnormality in the process and inform it to the plant personnel as soon as it occurs preventing run-away situations.

We have successfully developed software using the batch historical data given by HEMRL. The appropriately tuned software is successfully installed at HEMRL and its use was demonstrated for online plant data.



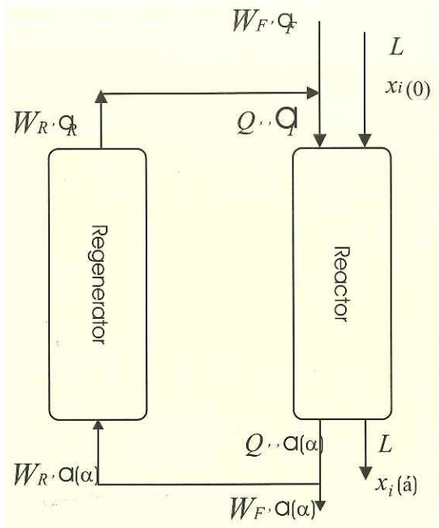
Idea of Kernel PCA: Mapping of data to Feature space F with function $\hat{O}$ and perform linear PCA in the feature space.

Modeling and simulation of catalytic reactions and reactors including their deactivation patterns

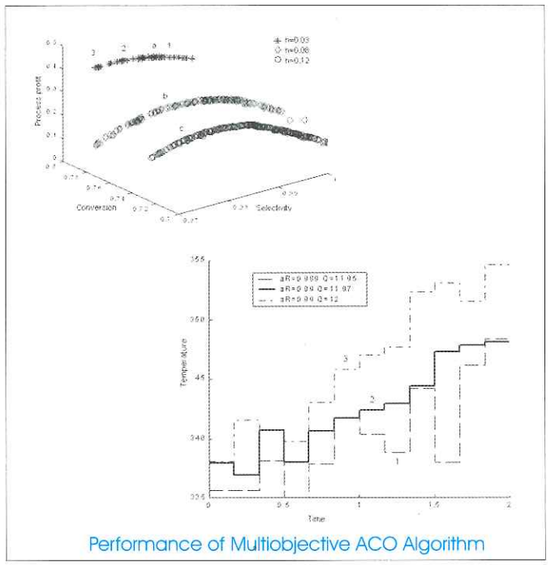
This work focuses on the development of a multi-objective optimization algorithm for a tubular reactor-regenerator system with a moving deactivating catalyst. The task is to find the optimal temperature profile along the tubular reactor, catalyst recycle ratio and the regeneration capacity for maximizing the process profit flux, selectivity and conversion. As the existing deterministic methodologies are best with convergence difficulties we employed

Food Search Process of Real Ant Colonies Double Bridge Experiment

The ***Ant Colony Metaheuristic*** for the multi-objective optimization. The software agents deputed for finding the optimal reactor conditions are inspired by the cooperative search behavior of real life ants. The algorithm was able to produce the complete spectrum of non-dominated solutions for the problem. The algorithm is very robust and computationally easy to implement.



Concurrent tubular reactor-catalyst regenerator system



Performance of Multiobjective ACO Algorithm

3.4 Artificial intelligence formalisms

Artificial Intelligence (AI) methodologies have opened up an attractive avenue for modeling, classification, monitoring and optimization of complex nonlinear systems, which are not easily amenable to conventional techniques. Accordingly, several AI formalisms for developing new modeling and optimization strategies for a variety of chemical, biological and chemical

engineering/technology systems have been applied (see Table).

AI formalism	Application area
Artificial neural networks (ANNs), Genetic programming	Modelling of batch/continuous catalytic, polymeric, biochemical, and biological processes, Development of soft-sensors
Feed forward and generalized regression neural networks (GRNNs)	Process monitoring and fault detection and diagnosis
Artificial neural networks and Fuzzy logic	Control of nonlinear processes
Genetic algorithms	Robust optimization of laboratory, pilot-plant and commercial scale processes in the absence of phenomenological models

3.4.1 Artificial neural networks

ANNs offer several advantages for developing process models: (i) the model can be constructed solely from the historic process input-output data, (ii) detailed knowledge of process phenomenology (kinetics, thermodynamics, mass/heat transfer mechanisms, etc.) is not essential for the model development, (iii) A properly developed model possesses excellent generalization ability owing to which it can accurately predict outputs for a new input data set and (iv) even multiple input - multiple output (MIMO) nonlinear relationships can be approximated simultaneously. Due to their several attractive features, ANNs for a wide variety of chemical engineering/technology applications have been applied for i) development of soft-sensors (software based sensors) for a commercial polyethylene process, ii) process identification and model based nonlinear control of zeolite catalyzed phenol to dihydroxybenzenes hydroxylation process, iii) modelling of batch polymerization reactors, and iv) batch and continuous process monitoring using generalized regression neural networks (GRNNs)

3.4.2 Genetic programming

The Genetic programming (GP) formalism is a novel but the least-studied artificial intelligence based modeling technique, which performs symbolic regression (SR). SR is a process of discovering both the mathematical form of a data-fitting function and all of its necessary coefficients (parameters). Thus, the GP methodology is capable of automatically obtaining the mathematical equation that fits a given set of process input-output data. The GP-based methodologies developed are: i) monitoring of bioprocesses: application to continuous production of gluconic acid by immobilized *Aspergillus niger*, ii) identification of pH control process, and iii) modelling of glucose to gluconic acid fermentation.

3.4.3 Genetic algorithms

The Genetic algorithms (GA) are ideally suited for solving complex optimization problems involving very large search spaces. The principal features possessed by the GAs are: (i) they require only scalar values and not the second- and/or first-order derivatives of the objective function, (ii) capability to handle nonlinear and noisy objective functions, (iii) GAs perform global search and thus are more likely to arrive at or near the global optimum, and (iv) GAs do not impose pre-conditions, such as smoothness, differentiability and continuity, on the form of the objective function. Due to their attractive features, the GAs have been employed for optimizing a number of chemical/biochemical systems, namely: i) optimization of TS-1 catalyzed hydroxylation of benzene process, ii) optimizatinon of benzene isopropylation on Hbeta catalyst process, iii) optimization of glucose to gluconic acid fermentation, and iv) optimization of batch and continuous distillation columns.

3.4.4 Hybrid AI methodologies

The AI-based modeling formalisms namely, artificial neural networks and genetic programming, and the optimization paradigm viz. genetic algorithms, though are powerful individually, their potential can be leveraged maximally by hybridizing them. Accordingly, two novel hybrid modeling-optimization schemes namely, ANN-GA and GP-GA have been developed. In these methodologies, an ANN or a GP based process model is optimized using the GA method. The significant advantage of these hybrid approaches is that process modeling and optimization can be performed exclusively from the historical process input-output data.

Hence, it is not necessary to develop a phenomenological model which in general is a difficult, cumbersome and costly task for optimizing a process. Using the hybrid strategies, it is possible to simultaneously obtain the optimal values of process operating variables and also their tolerances, which effect improvements in the process performance. The proposed hybrid methodologies have been successfully employed for the modeling and optimization of catalytic and biotech processes namely: i) TS-1 catalyzed hydroxylation of benzene, ii) non-isothermal continuous stirred tank reactor (CSTR), and iii) glucose to gluconic acid fermentation.

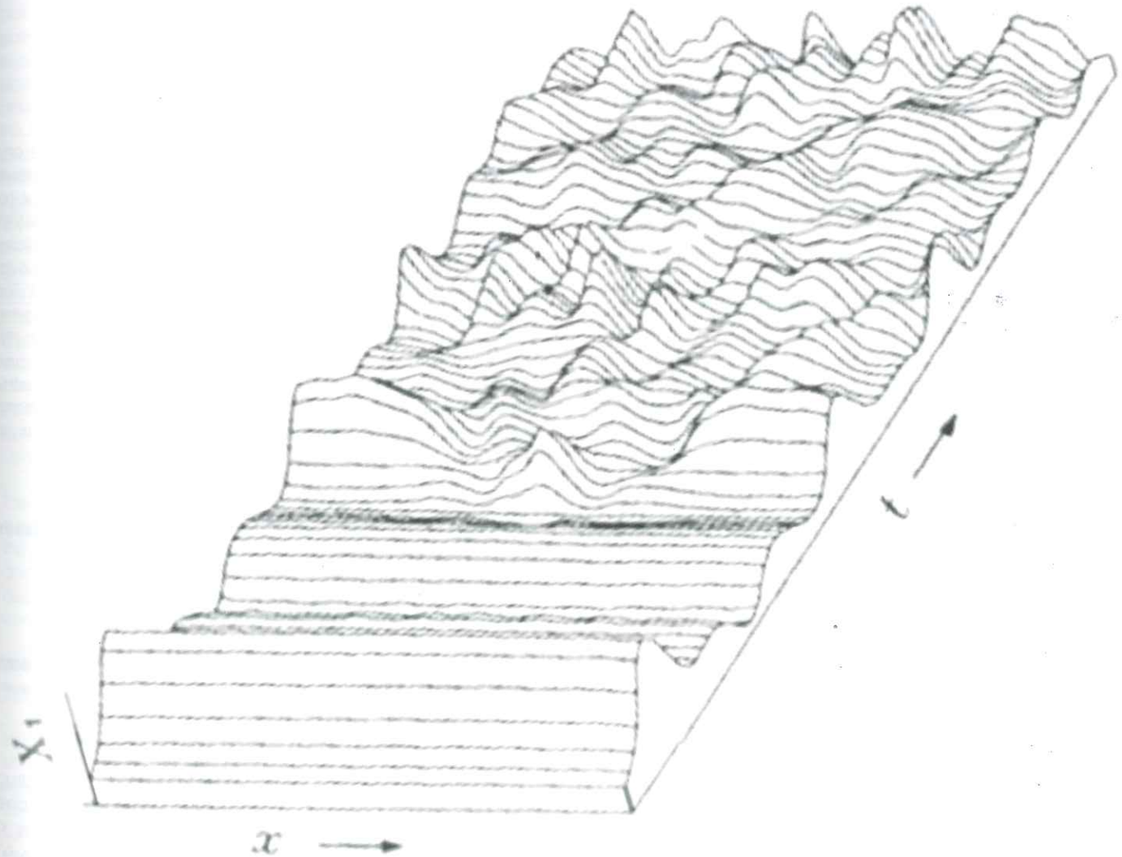
3.4.5 Artificial neural network based models for polyethylene plants

The objective of this project was to develop artificial neural network (ANN) based soft-sensor models for predicting three polyethylene (PE) quality variables, namely, melt flow index, stress exponent and density. This work was carried out in two phases. Specifically, 22 soft-sensor models pertaining to various catalyst operating modes and feed stocks were developed. For the two polyethylene plants (PE-I and PE-II). The extensive historic process data used in the development of soft-sensors were provided by the sponsoring industry. Since process data contained instrumental and measurement noise, a novel formalism was invented to increase the prediction and generalization ability of the soft-sensor models. This formalism has yielded soft-sensor models possessing very high prediction and generalization abilities.

The optimal soft-sensor models that were developed have been deployed on the distributed control systems (DCS) of the commercial scale PE plants. User-friendly software in C language was developed for this purpose. It fetches process operating variable values from the DCS and makes almost instantaneous predictions of the three QC variables. The software also has a provision to extract that historic process data, which closely match with the current process conditions.

3.4.6 Artificial neural network based modeling of food processes

Principal objective of this project was to develop ANN based models for evaluating quality attributes of two mass consumer products namely tea and "ready-to-eat" chapatis *(round flat unleavened bread made from wheat flour)*. Specifically, ANN



(A and B) corresponding to the teas originating from two Asian countries including India. The objective of modeling, which was accomplished successfully, involved development of ANN-based models for predicting the tea quality attributes such as flavor and liquor.

based models were developed using two input-output data sets an extensive data analysis and ANN-based modelling work was conducted on the wheat dough - chapati data. The inputs to the ANN model were the values of various chemical constituents of wheat dough that were determined by analytical and instrumental methods. Based on these inputs, the ANN model predicted the outputs describing quality variables of chapati namely, pliability, chewability and tearability. The ANN models developed under this project have a potential usage in maintaining quality of the food products.

4. Organic chemistry

4.1 Process chemistry

Synthesis of novel flame retardant additives

Flame retardant additives based on triazinyl borates, arylsulphonylamino triazines and borates of neopentyl alcohol, pentaerythritol, trioctanol and triethanolamine were synthesized and fully characterized by spectral and elemental analyses.

Synthesis of monomers

The monomer 4-{4-{4-[4-formyl-cycloheaxecarbonyl)-amino]-cyclohexylmethyl}-cyclohexyl carbamoyl) cyclohexanecarboxylic acid methyl ester was prepared by the condensation of 4,4-diaminocyclohexyl methane and 4-chlorocarbonyl-cyclohexane carboxylic acid methyl ester in the presence of triethyl amine. It was fully characterized by spectral and elemental analyses. The process has been scaled up to synthesize 500g of the material.

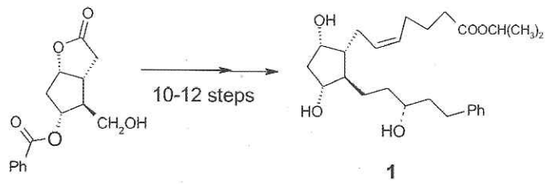
4.1.1 Chiral drugs

Process development for the drug Cialis

A laboratory scale process for the drug Cialis was developed. Cialis is the oral Phosphodiesterase type 5 (PDE5) inhibitor prescribed for the treatment of erectile dysfunction (ED). Cialis belongs to a class of pyrido-indole derivative (6R,12aR)-5-(1,3-benzodioxo-5-yl)-2-methyl-1,2,3,4,6,7,12,12a-octahydropyrazino(2',1':6,1)pyrido(3,4-b)indole-1,4-dione. The synthetic sequence involves cyclization of D-tryptophan methyl ester with piperonal, separation of cis isomer, acylation with chloroacetyl chloride followed by reaction with methyl amine.

Process development for the prostaglandin analogue latanoprost

Latanoprost (**1**) is a prostaglandin analogue used as antiglaucoma agent. A laboratory scale process has been developed starting from Corey's lactone alcohol which involves about 10 to 12 steps including two Wittig reactions and stereoselective ketone reduction as key steps.



1

(R)Salbutamol hydrochloride and (R)Salbutamol sulfate

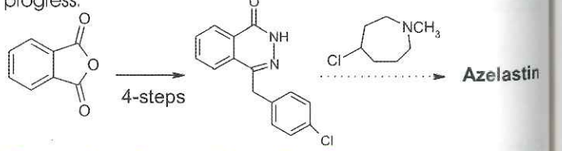
Racemic salbutamol (albuterol) is one of the most commonly used bronchodilators in the treatment of reversible airways obstruction. Racemic salbutamol comprises equal proportions of two isomers: (S)salbutamol and (R)salbutamol, with the latter being exclusively responsible for the activation of β-adrenoceptors. Within racemic salbutamol, it is (R)salbutamol that efficiently relieves obstruction of asthmatic airways and affords highly effective protection from bronchoconstrictor stimuli, including allergens. Increased hyperactivity after regular use of racemic salbutamol in patients with asthma is the result of a gradual accumulation of (S)enantiomer in the lung. After oral or intravenous administration of racemic salbutamol, the (R)enantiomer is metabolized several times faster than the (S)-enantiomer. Pharmacokinetically, (R)-salbutamol exhibits near absolute conformational stability. Therefore, (R)salbutamol provides a novel approach to asthma therapy which combines bronchodilation and bronchoprotection with anti-inflammatory efficacy.

A state-of-the-art process for the manufacture of (R)-salbutamol sulfate and (R)-salbutamol hydrochloride has been developed. These are the two water soluble pharmaceutically acceptable salts of (R)-salbutamol. The process of (R)-salbutamol is more chemistry oriented. Since chiral intermediates are involved, drastic reaction conditions and drastic reagents cannot be employed while developing (R)-salbutamol process. The critical stage of separation of (R)-and (S)-chiral intermediates has been worked out. The process has been transferred for commercialization to the industrial collaborator, who has started manufacturing (R)-salbutamol based on NCL's process.

4.1.2. Achiral drugs

Synthesis of antiasthamatic drug azelastin

Bench scale optimization of Azelastin, an antihistamine and antiasthamatic drug was undertaken. The synthetic route involved synthesis of two key intermediates viz. 4-(p-chlorobenzyl)-1(2H)-phthalazinone and 4-chloro-N-methyl-hexahydroazepinone. Condensation of these intermediates should provide azelastin. Optimization of preparation of 4-(p-chlorobenzyl)-1(2H)-phthalazinone has been completed. The second intermediate was attempted by several routes starting from N-methyl-β-alanine nitrile, methyl 3-(N-methyl)aminopropionate, 1,3,6-trihydroxyhexane and Dieckmann cyclization of N-(3-ethoxycarbonylpropyl)methyl amine which met with failures. Currently, Beckmann rearrangement of 4-hydroxy-cyclohexanone oxime is in progress.



Process development for roflumilast

A laboratory scale process has been developed for Roflumilast, an antiallergic/ antiasthmatic drug.

Process development for tenatoprazole

A laboratory process was developed for the drug tenatoprazole.The basic structure consists of one imidazopyridine ring and one pyridine ring bridged by a sulfinylmethyl chain. Chemically it is 5-methoxy2-(4-methoxy-3,5-dimethoxypyridine-2-yl methyl sulfinyl)imidazo (4,5-b)pyridine. The process was developed starting from commercially available 2,6-dichloropyridine.

4.1.3 Agrochemicals

Basic and strategic studies to commercialize hybrid wheat

This project was started with an objective of identifying right chemical hybridizing agents, utilize these to generate various hybrid seed varieties for wheat, and then commercialize these after large scale field trials at various centers spread over 8 wheat producing states representing various agroclimatic zones. Of the 160 compounds supplied by NCL, two were selected. Ten kg of these compounds were selected for winter crop season (2003). Large scale field trials are being conducted at sixteen different locations spread over eight states.

Synthesis of glucuronide conjugates

The main objective of the present investigation is the synthesis of glucuronide-herbicide conjugates and their use as pro-gametocides. β-Glucorinidase (GUS) is an enzyme that hydrolyses glycosidic linkage between β-glucuronic acidaglycon and is a foreigner for plants. However, recent developments in plant molecular biology allowed expressing this enzyme in plants with precise localization. Application of a glucuronide-herbicide conjugate on a plant where the GUS-enzyme has been expressed selectively in pollen should get hydrolyzed selectively and should release the latent herbicide. The released herbicide ultimately leads to the destruction of the pollen thus blocking the self-pollination. This methodology avoids use of active herbicide, which can cause a major damage to the plant and provides a site-specific release of herbicide. In this context, the synthesis of three different glucuronide conjugates of one of the identified herbicide asulam has been achieved. As this herbicide is not commercially available, a process for asulam with an overall 25% yield has also been developed. Initial studies showed the absence of herbicidal activity with three glucuronide conjugates synthesized.

The objectives of development of HPLC method for the evaluation of kinetic parameters and study of the hydrolysis of the asulam conjugates with acid as well as with glucoronidase and optimization of reaction conditions for the synthesis of asulam itself and also for the preparation of its glucuronide conjugates have been fulfilled.

Biodegradable pest control agents from non-edible oil seeds

Non-edible oil seeds have been known to exhibit a wide range of pest control activities like insecticidal, growth inhibition, repellent, antifeedant, attractant etc. Because of their biodegradability, efficacy and specificity to insects pests they form an important component of integrated pest management. Products prepared from the non-edible oil seeds viz neem *(Azadirachta indica)*, Karanja *(Pongamia glabra)*, Mahua *(Madhuca latifolia)* and Undi *(Calophyllum inophyllum)* were tested against pests of economically important crops, vectors and animal parasites.

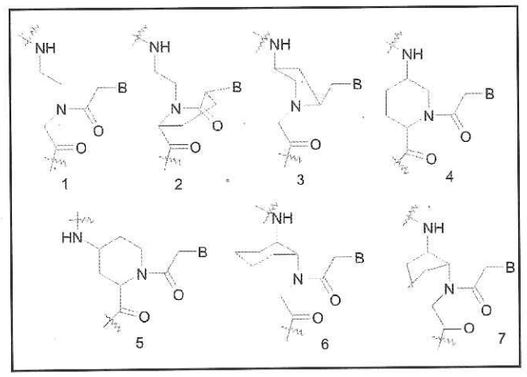
4.2 Bio-organic chemistry

4.2.1 Cyclitols

Progress in understanding of the role of cyclitols in cellular signal transduction, calcium mobilization, insulin stimulation, exocytosis, cytoskeletal regulation, intracellular trafficking of vesicles and anchoring of certain proteins to cell membranes is greatly aided by the availability of synthetic cyclitol derivatives and analogs. The key for the efficient synthesis of cyclitol derivatives is an understanding of the relative selectivity and reactivity of hydroxyl groups, which is dependent on inherent factors such as acidity of the free hydroxyl groups, hydrogen bonding and interactions with neighboring functional groups, and conformation of the carbocyclic ring. Work in NCL is towards delineating the reactivity pattern of hydroxyl groups of inositol derivatives and found to have C-1 (C-3)> C-4 (C-6)> C-5> C-2 in *myo*-inositol and *C-4 > C-2 ~ C-6 in myo*-inositol 1,3,5-orthoesters. The X-ray crystal structures of inositol derivatives provided important data for explaining or predicting the reactivity of hydroxyl groups. Discovery of inositol analogues, which could specifically interfere with signaling steps, would be of great use as biochemical tools as well as potential drug.

4.2.2 Peptide nucleic acids

Among various DNA analogues,peptide nucleic acids (PNA) **(1)** is emerging as a potential antisense agent. Continuing our studies on conformationally constrained peptide nucleic acids, several newer analogues have been designed, synthesized and evaluated for their biophysical properties toward hybridization with complementary oligonucleotides. The final aim is to screen different PNA analogues for higher affinity binding without losing sequence selectivity and impart DNA/RNA discriminating property. The PNA analogues studied include those with 5-membered pyrrolidine/one (2,3) and 6-membered pipecolic acid hybrids (4,5) and the cyclohexyl/ cyclopentyl fused backbones (6,7). Some of these analogues have shown desirable attributes of superior binding without loss of sequence selectivity and some preference in DNA/RNA binding attributes.



4.2.3 Collagen mimetics

Collagen is the most abundant structural protein in mammals and its mechanical properties are related to the high thermal stability of its triple helical structure. The primary structure of collagen is characterized by a repeating triplet (Pro-Hyp-Gly)

collagen. by replacing Hyp with 4-aminoproline it was demonstrated that the derived collagens form more stable triplexes. The stereo and positional dependence of aminoproline on triplex properties of collagen is being investigated. Apart from understanding structure-property relationships, the results have a direct bearing on novel applications of collagen analogues in cosmetics and healthcare.

4.2.4 HIV Tat1-NFκB interaction

HIV-1 Tat protein reprograms cellular gene expression of infected as well as uninfected cells apart from its primary function of trans-activating HIV-1 long terminal repeat (LTR) promoter by binding to a nascent RNA stem loop structure known as transactivator response region (TAR). Tat also induces chromatin remodeling of proviral LTR mediated gene expression by recruiting histone acetyl transferases (HATs) to the chromatin, which results in histone acetylation. Furthermore several studies have shown convincing evidences that Tat can transactivate HIV-1 gene expression in absence of TAR, the molecular mechanism of which remains to be elucidated. A direct interaction of Tat with nuclear factor kappa B (NFκB) enhancer, a global regulatory sequence for many cellular genes both *in vitro* and *in vivo* has been demonstrated. This interaction not only provides a novel molecular basis to explain TAR independent transactivation in HIV-1, but also points towards the potential mechanism of Tat mediated modulation of cellular genes.

4.3 Organic synthesis

Enantioselective synthesis of biologically active compounds

Asymmetric synthesis is one of the most fascinating areas of research in organic synthesis. Among an array of naturally occurring and biologically important compounds, the amino alcohols and lactones occupy a prominent position. The strategy features Sharpless asymmetric dihydroxylation routes to the various target compounds. Thus the synthesis of enantiomerically pure phenylephrine hydrochloride, (-)-conhydrine, (-)-acaterin, (S)-oxybutynin, R and S-massoialactone has been accomplished. The concept of double diastereoselection in asymmetric dihydroxylation has been successfully utilized for the total synthesis of phytosphingosine.

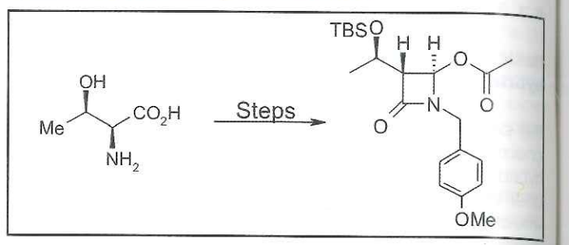
Synthesis of biologically active compounds

Syntheses of saintopin, combretastatin analogues, rebeccamycin and its analogues, optically active terrain and podophylotoxin analogues are in progress.

Synthesis of 2-alkylcysteine and 2-(hydroxylatedphenyl)-4-alkylthiazoline-4-carboxylic acids and derivatives

The methods for preparing 2-alkylcysteine derivatives, many of which can be performed stereoselectively, were developed. Likewise preparatory methods for the synthesis of a class of iron-chelating agents related to desferrithiocin, all of which containing a thiazoline ring have been evolved.

Synthesis of 4-acetoxy-2-azetidinone



Starting from natural amino acid the synthesis of 4-acetoxy-2-azetidinone as shown has been achieved.

Synthesis and screening of ionic liquids and their utilization in useful organic transformations

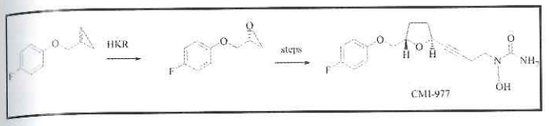
Minimizing downstream effluents and volatile organic compounds contents in atmosphere are the most important steps towards the "Green Chemistry". Ionic liquids (ILs), a developing area to address the goals of clean reactions by virtue of non-volatility, thermal stability and recyclability, will occupy a prominent place as a substitute for presently used volatile organic solvents. The objective of present investigation is to screen a number of ILs for industrially important organic transformations which may also confer additional benefits of enhancement in reactivity and selectivity. Several ILs based on 1-n-alkyl imidazolium, 1,3-n-dialkyl and N-butyl pyridinium salts have been synthesized. Characterization of ILs by spectral and elemental analyses have been carried out. A novel route to the synthesis of 2-substituted aryl-4-(H)-quinolines using IL under ambient conditions has been developed. Room temperature IL promoted regioselective synthesis of 2-aryl benzimidazoles benzoxazoles, benzthiazole and 1,5-benzodiazepines under ambient conditions have been developed.

Design, synthesis and application of new flexible three dimensional templates: a modular approach to pre-fabricated biomolecular segments

An important objective in modern synthetic and medicinal chemistry concerns the design of synthetic models that mimic various aspects of biologically active molecules. Detailed study of such models could lead to the development of better chemo-therapeutic agents, novel artificial restriction enzymes and molecular biological and diagnostic tools. There is currently considerable interest in the design and synthesis of various templates that can be used as structural mimicking portions of biologically active molecules. Majority of these templates are either rigid planar, conformationally fixed bicycles or some times acyclic skeletons with stereo chemical modulators. The prime objective of this project is to design and synthesis of flexible three dimensional templates and their further execution as modular frame works for mimicking the secondary structures of biopolymers. Work in the direction of the synthesis of the designed templates is in progress.

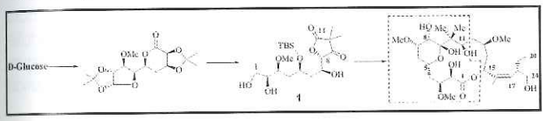
Asymmetric synthesis of CMI-977 (LDP-977): A potent anti-asthmatic drug Lead

Enantioselective gram scale synthesis of CMI-977 has been described using the tandem sequence of α-chloroepoxide fragmentation and intramolecular nucleophilic substitution as the key step. Combination of Jacobsens hydrolytic kinetic resolution and Sharpless asymmetric epoxidation were explored on the way to achieve the key intermediate.



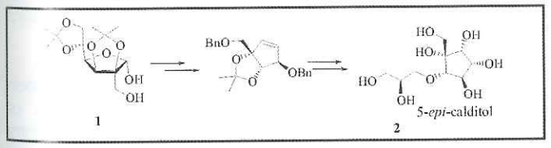
Toward a synthesis of the antitumor macrolide peloruside A: A chiral pool approach for the C(1)C(11) segment

A chiral pool approach starting from D-glucose involving RCM and stereoselective dihydroxylation as key steps, addressed the synthesis of **1**, an advanced intermediate corresponding to the C(1)-C(11) portion of peloruside A.



Stereoselective synthesis of 5-epi-calditol

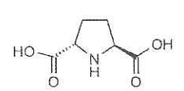
Intrigued by the structural similarity between the cyclopentitol moieties of various natural products, a program is initiated towards the synthesis of these subunits preferably using a common starting point. The preliminary work in this direction involved the synthesis of a differentially protected cyclopentitol derivative **1**, its stereoselective dihydroxylation and conversion of the resulting diol into 5-*epi*-calditol **2**.



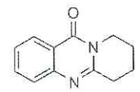
4.3.1 Total synthesis

Total synthesis of bioactive natural products occupies keystone position in organic chemistry. Total synthesis of several complex bioactive natural, unnatural, pseudo natural and hybrid natural products using variety of new, elegant synthetic strategies is being currently perused.

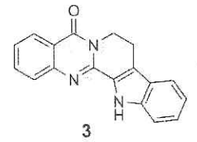
Some of the natural products synthesized includes (2*S*, 5*S*)-pyrrolidine-2,5-dicarboxylic acid (**1**), mackinazolinone (**2**), rutaecarpine (**3**) (antihypertensive), pulchellalactam (**7**) (CD45 PTP inhibitor), remotely functionalized alkylmethylmaleic anhydrides (ras farnesyl protein transferase inhibitor) (**4-6**), salfredin B_{11} (**10**) (aldose reductase inhibitor), phthalidochromine (**8**), CJ-13,015 (**9**) (Anti-***Helicobacter pylori***), 2-carboxymethyl-3-hexylmaleic anhydride (**5**), 2-(β-carboxyethyl)-3-octylmaleic anhydride (**6**) and luotonin A, B & E (**11**, cytotoxic). Synthesis of salfredin-B_{11} was achieved via novel regioselective condensation of 3,5-dihydroxyphthalide with prenal. A remarkably tuned regioselective quinazolinone directed *ortho*-lithiation on adjacent quinoline moiety has been used as a key step for short and efficient synthesis of human DNA topoisomerase I poison luotonin A, (IC_{50} 5.7-12.6 μm/mL) and luotonin B & E.



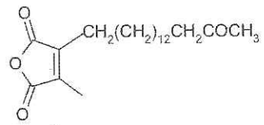
1
(2*S*,5*S*)-Pyrrolidine-2,5-dicarboxylic acid



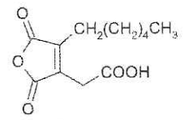
2
Mackinazolinone



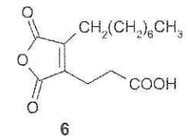
3
Rutaecarpine



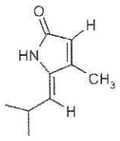
4
Remotely functionalised alkylmethylmaleic anhydride



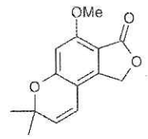
5
2-Carboxymethyl-3-hexylmaleic anhydride



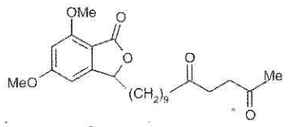
6
2-(ß-Carboxyethyl)-3-octylmaleic anhydride



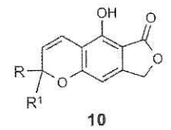
7
(Z)-Pulchellalactam



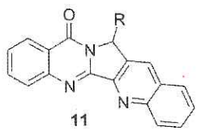
8
Phthalidochromine



9
CJ-13,015



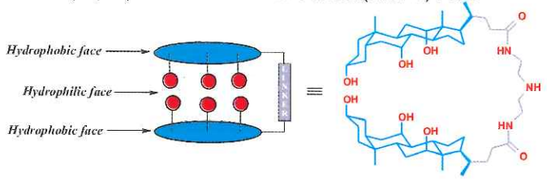
10
Salfredin B_{11}



11
Luotonin A: R = H
Luotonin B: R = OH

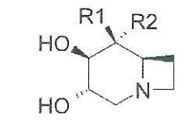
New steroidal dimers with antifungal and antiproliferative activity

Bile acid-derived novel amphiphilic dimers were synthesized and tested for antifungal and antiproliferative activity *in vitro*. These were found to be active against *C. albicans, Y. lipolytica,* and *B. poitrassi* at nanomolar concentration without effect on cell proliferation. They also inhibited the growth of human oral cancer (HEp-2) and human breast cancer (MCF-7) cells.

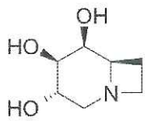


Photoinduced electron transfer (PET): Applications in organic synthesis

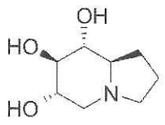
Utilizing PET mediated amine radical cations for constructing cyclic amine, new conformationally restricted glycosidase inhibitors **1** which mimic the transition state of glycosidic bond cleavage or formation, polyhydroxyazepines (**8,9**), castanospermine analogues (**2-4**) and (+)-7-deoxypancratistatin (**5**) a potent anti neo-plastic agent have been synthesized. (±)-Pancracine (**6**) was synthesized by the [3+2] cycloaddition of the non-stabilized azomthine ylide precursor. *trans*-Hydrindane (**7**), which forms a common feature of various higher terpenes, steroids and vitamin D was synthesized from the cheaply available aromatic compounds using Birch reduction, alkylation and Claisen rearrangement as the



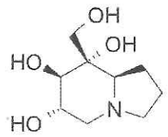
1



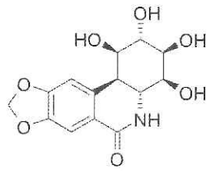
2



3

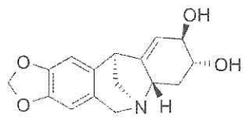


4



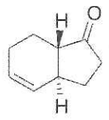
5

(+)-7-deoxypancratistatin

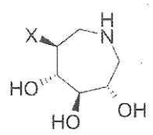


6

(±)-Pancracine

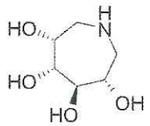


7



8

X = OH, CH_3



9

Total synthesis of thia-calanolide

Total synthesis of racemic Thia-Calanolide has been undertaken and the work is nearing completion. Calanolide A is an established anti-HIV drug isolated from natural sources. Its synthetic analogue aza-calanolide was found to be more active than Calanolide A itself. This prompted us to undertake the total synthesis of thia-calanolide, the sulphur analogue. Various intermediates in the synthesis as well as thia-calanolide will be subjected to testing as an anti-HIV agent.

Utilisation of olefin metathesis and ring closure metathesis towards the synthesis of antitumour alkaloids and natural products

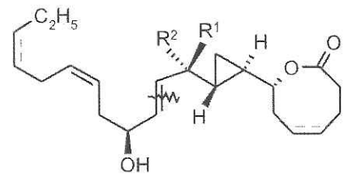
The main objective of the present investigation is to utilize olefin metathesis reaction for the synthesis of antitumour alkaloids and natural products. The molecules undertaken were anticancer compounds like camptothecin, mappicine ketone, homocamtothecin, etc. by utilizing the metathesis reaction for the construction of D ring of camptothecin, synthesis of olefins by cross olefin metathesis as well as enyne metathesis.

The efficacy of ring closing metathesis reaction has been established for the synthesis of key D ring skeleton of camptothecin and mappicine ketone and formal total synthesis of camptothecin has been accomplished and a novel protocol of 1,4-addition of nitroalkanes to unactivated α,β–unsaturated lactam has been accomplished. Total synthesis of camptothecin and mappicine ketones and other alkaloids is in progress.

Ring-closing metathesis (RCM) reaction: Application in the synthesis of cyclopropyl-lactone segment of solandelactones

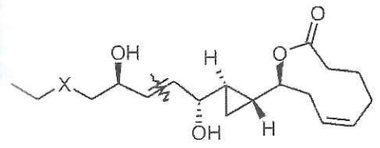
The formation of rings represents a central theme in natural product synthesis. A number of natural products contain medium-sized saturated as well as unsaturated lactone rings. This class of compounds continues to generate intense interest from synthetic organic chemists due to their interesting structural features associated with important biological activities. Usually, medium sized lactone rings are achieved by Yamaguchi lactonisation under high dilution condition or Bayer-Villiger ring

expansion reaction. In order to facilitate the formation of medium-sized rings, several features should be installed in the substrate so that it can provide some sort of conformational constraint or restraint. For example, under Yamaguchi condition, the eight- and nine-membered lactone rings corresponding to solandelactones and halicholactone respectively were facilitated by the presence of *cis*-alkene conformational restraint. Synthesis of medium sized rings by RCM reaction using Grubbs' catalyst is a formidable challenge despite the use of this methodology for the construction of diverse medium sized cyclic structures. Because of the enthalpic as well as entropic influences, eight-membered lactone rings are the most difficult to prepare. The application of RCM reaction has been described as flexible approach towards the synthesis of saturated and unsaturated eight-membered lactone rings present in solandelactones.

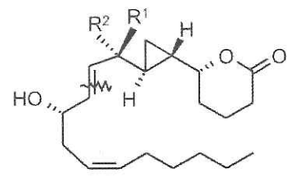


R^1 = H, R^2 = OH; R^1 = OH, R^2 = H

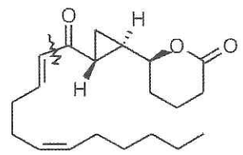
1. Solandelactones A-H



2a. X = -CH_2-CH_2- (Halicholactone)
2b. X = cis-CH:CH (Neohalicholactone)



3a. R^1 = H, R^2 = OH; Constanolactone A
3b. R^1 = OH, R^2 = H; Constanolactone B



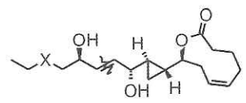
4. Eicosanoid

Solandelactones (**1**) belonging to the growing class of oxylipins containing a *trans*-bifunctional cyclopropane ring and fatty acid lactones of marine origin were isolated from the hydroid *Solanderia secunda* of Korean waters and their structures were elucidated by exhaustive spectroscopic and chemical method. Their structural uniqueness as well as intriguing biological activities led us to synthesize them in a suitable manner. These compounds were found to be structurally similar to some other marine oxylipins *viz* constanolactones (**3**), halicholactone (**2a**) and neohalicholactone (**2b**). It is interesting to note that all of the above metabolites possess linear C_{20} carbon skeletons derived from eicosanoid origin. In contrast, solandelactones with saturated and unsaturated eight-membered lactone rings and C_{22} carbon skeleton are thought to be of docosanoid precursor.

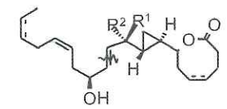
An efficient synthesis of cyclopropyl-lactone containing fragment of solandelactones has been achieved via ring-closing olefinic metathesis reaction. Grubbs' second generation $RuCl_2(=CHPh)(PCy_3)$(IEMS) catalyst has been successfully and efficiently utilized in the construction of eight-membered lactone ring with *cis*-double bond present in solandelactones.

Chemo-enzymatic total synthesis of eicosanoid

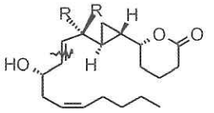
As a part of defense mechanism, marine organisms produce a fascinating range of secondary metabolites endowed with unusual and unexpected biological profiles. The arachidonic acid (AA) pathway in marine organisms provided a number of oxylipins such as **1-3** containing the cyclopropyl-lactone groups. Eicosanoid (**4**) was isolated by the incubation of arachidonic acid with an acetone powder of the Caribbean soft coral *Plexaura homomalla*. In conjunction with other marine fatty acid metabolites, eicosanoid **4** also incorporate a cyclopropane-lactone motif and lipoxygenase inhibiting activity and therefore provoked a considerable synthetic interest. It is likely that the origin of eicosanoid **4** might have occurred from transformation analogous to that as constanolactones **3**. To expedite current pharmaceutical evaluations of this family, an asymmetric total synthesis of eicosanoid **4** has been described. The synthetic protocol involved modified Simmon-Smith cyclopropanation, enzymatic resolution of homoallyl alcohol, ring closing metathesis (RCM), and Nozaki-Kishi coupling reaction.



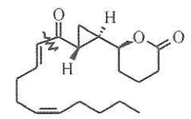
1a, X = -CH_2-CH_2- (Halicholactone)
1b, X = cis-CH:CH (Neohalicholactone)



R^1 = H, R^2 = OH; R^1 = OH, R^2 = H
2, Solandelactones A-H



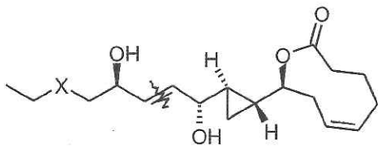
3a, R^1 = H, R^2 = OH; Constanolactone A
3b, R^1 = OH, R^2 = H; Constanolactone B



Eicosanoid **4**

Studies on the total synthesis of halicholactone and neohalicholactone: A stereoselective synthesis of C1-C13 fragment

Secondary metabolites halicholactone (**1a**) and neohalicholactone (**1b**) showing lipoxygenase inhibitor activity were isolated previously from the marine sponge *Halichondria okadai*. The elegant structural and stereochemical features of halicholactone (**1a**) and neohalicholactone (**1b**) decorated with dense functionalities that include an unsaturated nine-membered lactone, a *trans*-disubstituted cyclopropane ring and five stereocenters present a considerable challenge as synthetic targets, particularly with respect to stereochemistry and functional group sensitivity, attracted our attention to undertake its synthesis. Although, a few number of partial and total synthesis have been reported, the stereoselctive construction of the stereogenic centers of C-9 to C-12 is still remained to be solved.



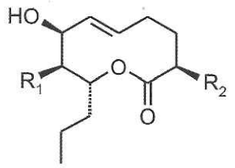
1a, X = -CH_2-CH_2- (Halicholactone)

1b, X = cis-CH:CH (Neohalicholactone)

A synthetic strategy, which allows complete stereochemical control of all four stereocenters (8S, 9R, 11R, 12R) of cyclopropyl and lactone containing fragment of halicholactone **(1a)** and neohalicholactone **(1b)** starting from l-isopropylidene synthesized has been devised.

First total synthesis of herbarumin III

The interesting biological activities of herbarumin I (**2**) and II (**3**), reinvestigation of the fermentation broth and mycelium of the fungus *Phoma herbarum* led to the isolation of a new phytotoxic nonenolide (7*R*,9*R*)-7-hydroxy-9-propyl-5-nonen-9-olide, (herbarumin III, **1**), along with two known compounds herbarumin I (**2**) and II (**3**). The structure of **1** was elucidated by spectroscopic method combined with molecular modeling. Compounds **1** to **3** interacted with bovine-brain calmodulin and inhibited the activation of the calmodulin-dependent enzyme camp phosphodiesterase.



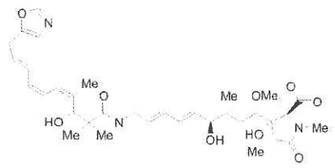
1. R_1 = R_2 = H (Herbarumin III)
2. R_1 = OH, R_2 = H (Herbarumin I)
3. R_1 = R_2 = OH (Herbarumin II)

In general, the synthetic approaches to lactones have been focused mainly on the use of fragmentation /ring expansion reactions and on lactonization strategies in order to build the lactone ring. Ring-closing metathesis (RCM) is a modern synthetic protocol to design various lactone rings. The total synthesis of herbarumin I (**2**) and herbarumin II (**3**) have been recently reported following RCM or Nozaki-Hiyama-Kishi reaction as the key step. Our synthetic strategy for the total synthesis of herbarumin III (**1**) hinges on the RCM reaction as a key step for lactone ring formation with envisaging the required chiral aliphatic diol to arise from the D-glucose.

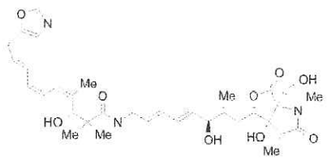
First total synthesis of biologically active natural product herbarumin III (inhibits the activation of the calmodulin-dependent enzyme camp phosphodiesterase) starting from cheaply available D-glucose in a concise and efficient manner has been achieved.

Synthetic study towards the spiro-bicyclic-β-lactone segment of oxazolomycin

Oxazolomycin (**1**) and neooxazolomycin (**2**) were isolated from the strain of *streptomyces* sp. KBFP-2025. They were earlier characterized by strong antibacterial and anticancer activities. Later studies found them to possess exceptional abilities to suppress the replication of vaccinia, herpex simplex virus type-1 and influenza A virus during one step grown cycle experiments in both human and chicken cells. The unique structural feature of **1** is the spiro-bicyclic-β-lactone structure whose synthesis was reported on a model compound by Taylor et al. The basic premise of their synthesis was to construct the spiro-β-lactone ring on a pyrrolidine precursor followed by the oxidation to pyrrolidinone.



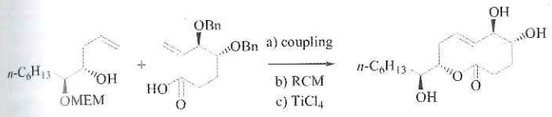
Oxazolomycin (**1**)



Neooxazolomycin (**2**)

The stated objective of methodology is to adopt the Evan's aldol reaction leading to the 3,4-disubstituted-prolinol intermediate. To install the spiro-β-lactone ring, cross-Cannizzaro reaction would be envisaged while the pyrrolidinone skeleton could be realized by using Taylor's oxidation strategy. A synthetic strategy to prepare the novel spiro-bicyclic -β-lactone system present in oxazolomycin has been investigated. The construction of the spiro-β-lactone ring was accomplished using cross-Cannizzaro reaction while 3,4-disubstituted pyrrolidine ring, was prepared using Evan's aldol reaction.

Total synthesis of microcarpalide

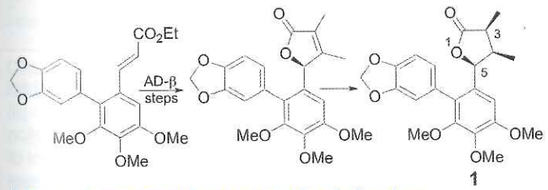


1

A total synthesis of microcarpalide (**1**), a potent microfilament disrupting agent has been described using ring closing metathesis as the key step. A blend of chiral pool approach and asymmetric dihydroxylation has been executed for successful total synthesis of this natural product. The described total synthesis of microcarpalide in its naturally occurring form is characterized by a convergent strategy and considerable flexibility for the construction of related non-natural analogues for the structure activity studies.

Total synthesis of putative structure of eupomatilone-6

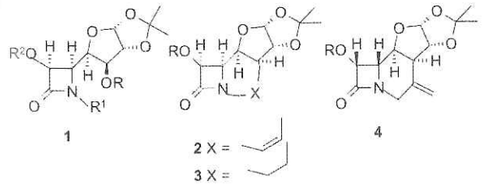
The synthesis of eupomatilone-6 (**1**) has been achieved by using the Suzuki coupling, Sharpless asymmetric dihydroxylation and intramolecular Horner-Wadsworth-Emmons reactions. The spectroscopic studies carried out on synthetic eupomatilone-6 do not agree with those reported for the natural product and therefore revision of the assigned structure is warranted.



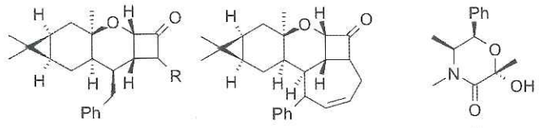
1

4.3.2. New synthetic methodologies

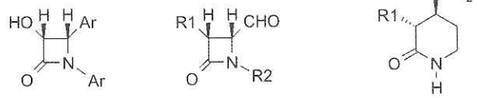
Asymmetric synthesis of *cis* β-lactams with very high diastereoselectivity by [2+2] cycloaddition of ketenes with chiral imines derived from D-(+)-glucose was developed for the synthesis of large number of substituted β-lactams (**1**). Renewed interest in novel bi- and polycyclic β-lactam systems to overcome bacterial resistance of β-lactam antibiotics has lead to the development of new synthetic approaches.



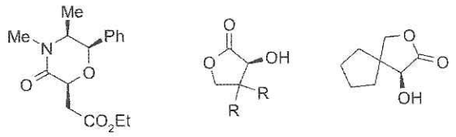
1 **2** X = **3** X = **4**



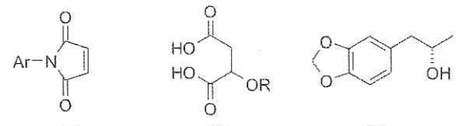
5 **6** **7**



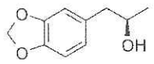
8 **9** **10**



11 **12** **13**



14 **15** **16**



17

Highly stereoselective and substrate-controlled synthesis of polycyclic β-lactams (**2-4**) from D-glucose derived chiral template *via* intramolecular free radical cyclization was developed. An efficient synthesis of pentacyclic β-lactams (**5, 6**) was achieved in high yield *via* a novel 6-*exo*-*trig*, 7-*endo*-*dig* tandem radical cyclization using (+)-carene derived chiral templates. Diastereoselective synthesis of β-lactams was achieved using chiral acid derived from (-)-ephedrine chiral template (**7**). Enantiopure 4-formylazetidin-2-ones (**9**) were used as building blocks for the synthesis of 4-aminopiperidin-2-ones (**10**) in very good overall yields. An efficient general route for the enantioselective synthesis of *S*-(+)-pantolactone and its analogues (**12**, **13**) was developed from an ephedrine-derived chiral morpholin-3-one (**11**).

A novel methodology for the preparation of dipyrromethanes and porphyrins was developed by using cation exchange resins as acid catalysts. Metallporphyrins and metallophthalocyanines anchored on various polystyrenes polymers were prepared for use as efficient catalysts in aerobic oxidation of alcohols. A simple, efficient and general two-step synthesis of

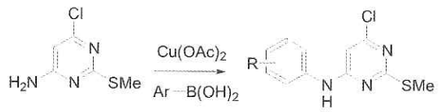
alkoxysuccinic acids (**15**), which involves base induced oxa-Michael addition to N-aryl maleimide **(14)** followed by acid hydrolysis, was developed. (*S*)-(+)-α-methyl-1,3-benzodioxole (**16**) and (R)-(-)-α-methyl-1,3-benzodioxole (**17**), a chiral building block for the synthesis of (-)-talampanel, was synthesized by Amano-PS catalyzed enantioselective acylation of racemic compound. N-Bromosuccinimide-dibenzoyl peroxide/azabisisobutyronitrile, as a new reagent for isomerisation of *Z*-alkene to *E*-alkene was developed. A direct one-pot method for the preparation of allyl azides from allyl alcohols using triphosgene was also developed.

Heterocyclization using ionic liquid as green solvent, promoter recyclable homogenous catalyst

The use of ionic liquids (ILs) due to their inherent acidity, promotes these heterocyclization reactions at ambient to mild reaction temperatures in enhanced reaction rates with high regio-selectivity without the need for any additional acid catalyst giving rise to easy work up procedures. Due to their non-volatability and thermal stability, the ionic liquids can be completely recovered and recycled into the process thus giving rise environment friendly technologies. IL have been used as reaction media, promoter and recyclable homogenous catalyst for heterocyclization and cyclocondensation reactions to generate heterocycles of commercial importance in diverse areas of uses such as quinolines, fused polycyclic quinolines and coumarins.

Copper-mediated coupling of aminopurines and aminopyrimidines with arylboronic acids

A general method for mono *N*-arylation of aminopurine and aminopyrimidines using an arylboronic acid and Cu(II) acetate has been developed.



3-Carboxy coumarins

A practical and environmentally friendly preparation of 3-carboxycoumarins has been developed starting from salicylaldehyde and Meldrum's acid. The condensation of salicylaldehyde with Meldrum's acid in water at 75°C leads to the formation of 3-carboxycoumarin derivatives.

Aziridination

A one-pot synthesis of 1,2-amino alcohols involving aziridination of alkenes followed by ring opening of the aziridines has been developed. A chiral version of the work is under progress. In continuation, a viable route to racemic aplha-methylcysteine has been developed starting from methylmethacrylate followed by aziridination and ring opening of the aziridine formed with thioacetic acid. Work on the extension of this methodology with different nucleophiles in the ring opening reaction is in progress.

Development of a laboratory scale process for the preparation of 3,3'-Diaminobenzidine

Diaminobenzidine (DAB) is an important monomer used for the preparation of membrane for fuel cell. A three step laboratory scale process for the production of DAB has been demonstrated. DAB is not available commercially in large quantities and is generally prepared from benzidine, its dichloro derivative, biphenyl etc. Existing methods for the production of DAB has the disadvantages like the use of benzidine the known carcinogens as the raw material, high temperature (200-300°C) and high pressure (900- 1000 psig) of the reaction, making the process more hazardous from safety and more reaction steps and low yield.

Two novel processes to obtain DAB of higher purity have been developed. In first process nitro-bromoacetamide (NBA) a non-carcinogenic raw material is used. The novelty of process is the use of palladacycles as a new efficient catalyst for the Suzuki type biaryls coupling of NBA to prepare intermediate 3,3'-dinitro-4,4'-diacetamidobiphenyl (DNDACB) from which DAB was obtained by known sequence of reactions (hydrolysis and reduction). The second method of preparation of DAB involves three- step process: oxidation of dichlorodiaminobiphenyl with novel catalyst Titanium Superoxide and hydrogen peroxide as oxidant and subsequent ammonolysis and reduction of the intermediate products. Both the processes have made it possible to obtain high pure DAB (100% purity). The process also has the advantages like: no by-products in the reaction mixture; heterogeneous catalysts used and reaction can be carried out at milder conditions of temperature (100°C) and pressure (100 psig).

4.3.3 Organometallic chemistry

Asymmetric catalysis using chiral metal complexes is an emerging area of modern organic chemistry. A variety of chiral Ti (IV) complexes were prepared and reduced to chiral Ti (III) complexes. These catalyze the pinacol coupling reaction stereoselectively. Ti-SALEN complex was found to be efficient at 10 mol % concentration. Chiral ruthenium complexes were prepared and used for selective transfer hydrogenation of aldehydes and ketones. Aziridination of olefins by chloramines-T, bromamine-T catalysed by cyclopentadienyl Ru (bis triphenyl phosphine chloride), Fe, Mn salen, $ZrOCl_2$, Fe (Phth), AuCl, $P(C_6H_5)_3$ in presence of NH_4BF_4, $AgNO_3$ were studied. Mizoroki-Heck reaction with new Pd-complexes was also studied. A new method for the reduction of azides and nitro compounds with $Mo(CO)_6$ was developed.

4.3.4. Bio-catalysis

Work on the biocatalysis using phosphorous based ionic liquids has been initiated. In the beginning, resolution of phenethyl alcohol by transesterification with vinylacetate using several commercially available lipases have been undertaken. The preliminary results are very encouraging.

4.4. Natural product chemistry

To achieve basic standardization of anti-diarrhoeal medicinal plants like *Karanj*, *Guava*, *Bael* and *Sunth*, their phytochemical evaluation has been undertaken concurrently with the biological assays employed. Different extracts of the above plants material were made and their HPLC profile was developed to detect drug active complex and attempt is being made to isolate the active components from the extracts by using different separation techniques.

Chemical investigation of medicinal plants

Two new and four known compounds have been isolated from the acetone and methanol extract of *Blainvillea latifolia* and characterized by spectral methods. Two new eudesmanolioks have been isolated from the aerial parts of *Sphaeranthus indius* and their structure determined by using modern spectral techniques. Three new sesquiterpene lactones have been isolated from the acetone extract of *Centratherum phyllolaneum* and structures were determined by Spectral methods. Two new and a known aromatic compounds have been isolated from the acetone extract of *Zingiber wightiana* and their structures were elucidated by spectral techniques.

Development and commercialization of bioactive substances from plant sources

A number of plants are used in different Indian traditional systems of medicines. This programme is aimed to collect selected traditional medicinal plants, prepare their extracts, test these extracts for different biological activities, identify the active principle(s) and initiate the work for the development of new single molecule drug/ standardized new herbal drug.

Different parts of plants (2nd and 3rd list by CSIR programme on development and commercialization of bioactive molecules from plant sources) have been collected and processed to prepare different extracts. These extracts have been submitted to thirteen CSIR laboratories for assaying them for their biological activities. Eighty extracts have been submitted for bioassay. A new list (4th list) of 25 plant species has been allotted to process under this programme of which 8 plant species available in good abundance in Western Ghats, have been collected and preparation of extracts of different parts of these plant material and submission for their bioassay is underway. A number of leads have shown promising activity and they are being followed further. The activities are as. Neurological disorders, 4 (to be tested for anti-parkinson's activity); Antidimensia, 17; Anti-anxiety, 11; Anti depressant, 1; Anti malarial, 6; Anti-TB,1; and Pesticidal, 1.

New natural products as HIV reverse transcriptase inhibitors from the genus *Calophyllum*

The genus *Calophyllum* has yielded a number of dipyranocoumarins which has exhibited HIV-RT inhibition activity. Of these coumarins calonolide A isolated from *C.lanigerum* is now a clinical drug for the treatment of AIDS. For the isolation of other coumarins exhibiting anti-HIV activity, investigation of different species genus *Calophyllum* available in Western Ghats has been initiated. Variation of bioactive molecules with respect progress. Chemical investigation of leaves of *C.apetalum* has yielded along with known dipyranocoumarin, a new natural product structure elucidation of which is in progress.

Bioprospecting with respect to genetic diversity of *Symplocos* and *Gaultheria* species

The three species of the genera *Gaultheria* and *Symplocos* have been found to have a wide variation in genetic diversity. Co-relation to this genetic diversity with chemical diversity particularly with respect to their bioprospecting has been taken up.

Leaf samples of *Gaultheria fragrantissima* from two biodiversity hotspot viz. North East Area and Nilgiris were collected by Botanical Survey of India. The genetic diversity of these plant samples were carried out and variation of essential oil (Wintergreen oil) of this plant material with respect to quality and quantity was carried out.

Results obtained show a distinct correlation of amount of oil present in the plant material with genetic diversity although it is necessary to analyse some more plant samples to conclude the results. Also efforts are being made to study seasonal variation with respect to quality and quantity of wintergreen oil. Chemical examination of *S. racemosa* leaf extract has been initiated.

Assessment and in vitro conservation of biodiversity in some guttiferous plant species of western ghats with special reference to development of bioactive molecules

Plant species belonging to the family Guttiferae are known to contain coumarins, xanthorides and triterpenoids. Some of these molecules are reported to possess wide range of biological activities like anti-viral (including anti-HIV), antifungal, anti-cancer anti-lipidogenic and pesticidal. The study biodiversity of the plant species belonging to the genus *Calophylum* with respect to bioactive molecules and their *in-vitro* conservation is important for the development of new bioactive molecules. Stem, leaves, fruits and bark of three species of *Calophyllum* viz. *C.inophyllum C.apetalium* and *C.polyanthum* were collected and extracted with two solvents each. Chemical examination of *C. polyanthum* for the isolation of compounds for using them as markers in the fingerprinting of the plant materials has been initiated. *In vitro* propagation of these plant species is being carried out.

4.5. Chemistry of colorants

Synthesis of novel colorants /intermediates

This exploratory program focuses towards the development of bright yellow, orange, violet, blue and blue-green chromophoric systems with improved photo stability, bleeding resistance and weatherability. This is being mainly sought to be achieved by incorporating functional UV stabilizers into the chosen chromophoric systems, improving compatibility by incorporating long alkyl chains and introduction of reactive groups into the chromophores which are capable of forming covalent bonds with the polymer back-bone in addition to the positioning of suitable auxochromes at appropriate places.

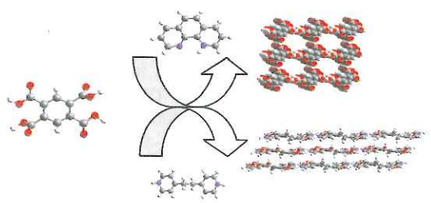
coumarin dyes were synthesized for further evaluation as colorants for plastics. In addition, several chromophores have been synthesized based on Disperse Yellow-44 analogues and Perylene dicarboximide derivatives to which functionalized UV stabilizers have been attached. The work is being continued in the same vein with essential functional UV stabilizers.

4.6. Supramolecular crystal engineering

Synthesis of supramolecular assemblies using the knowledge of intermolecular interactions such as hydrogen bonds is currently an area of frontier research, with a focus on developing catalysts with tailor-made properties and design of miniature circuits in the electronic industry etc. In this direction, development of cavity and channel structures have been done by employing molecules with functional groups such as -COOH, $-CONH_2$, $-NO_2$ etc that form robust hydrogen bonds. Studies were done on the development of polymorphs and pseudopolymorphs through various crystallization procedures.

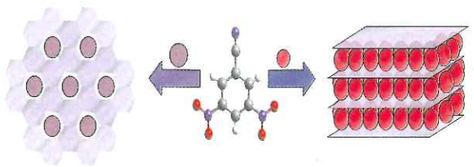
Assemblies of 1,2,4,5-benzenetetracarboxylic acid

Supramolecular assemblies of 1,2,4,5-benzenetetracarboxylic acid with *aza* donor molecules like 1,10-phenanthroline, phenazine, 1,7-phenanthroline, 4-(N,N-dimethylamino) pyridine, 1,2-*bis*(4-pyridyl)ethane and 1,2-*bis*(4-pyridyl)ethane with and without water were characterized by single crystal X-ray diffraction methods. These assemblies occur in two classes-host-guest systems (with aza molecules being in the channels created by the acid molecules) and assemblies with infinite molecular tapes.



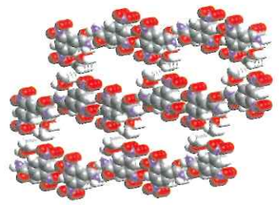
Assemblies of 3,5-dinitrobenzonitrile

In host-guest type complexes of 3,5-dinitrobenzonitrile with some hydrocarbons like benzene, naphthalene, o-xylene, and aza donor molecules (acridine, phenazine and phenothiazine), nitrile forms a host network, yielding channels (in three-dimensional arrangement), which are filled by guest molecules. In *p*-xylene complex, the nitrile and *p*-xylene are arranged with hydrocarbon embedded between the layers of nitrile, like in inorganic clay structures.



Assemblies of 3,5-dinitrobenzamide

3,5-Dinitrobenzamide and 4,4'-bipyridyl co-crystallize to yield different types of channel structure from methanol and water, constituting supramolecular pseudopolymorphs. While, in the methanol adduct, amide and methanol molecules form a double helix network, in the water adduct, amide and water molecules yield a planar layer structure. However, in both adducts, bipyridyl molecules sit in the channels created in the three-dimensional packing of the double helix or layers.



4.7. Entomology

Ultrastructural studies of chemosensilla on the antennae of *Trichogramma chilonis*, an egg parasitoid of *Helicoverpa armigera* and electrophysiolgical responses to volatile phytochemicals were evaluated. EAG profiles to the 22 chemicals reveal differences between males and females with oxygenated terpenes causing higher responses in females than in males where the fatty acid derivatives caused the highest response.

A number of plant extracts and oils sourced from NCL and other CSIR laboratories were screened for mosquito repellence, insect growth regulator, antifeedant, and insecticide and oviposition deterrence activities. The active fractions are now being taken to the next step of characterization.

5. Physical and materials chemistry

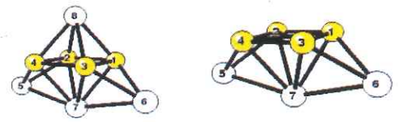
5.1 Theoretical Chemistry

5.1.1 Magnetic properties of molecules using coupled-cluster method

Coupled-cluster methods have emerged as state-of-the-art class of methods in the electronic structure, spectra and properties of closed-shell-like molecules. This efficiently takes care of the dynamic correlation arising out of electron-electron repulsion. Novel extended coupled-cluster (ECC) method, based on double-similarity-transformation, has been developed for the first time for calculation of response properties with respect to external perturbation. This has been used successfully for calculation of electric properties. This year, response of the ECC method has been studied with respect to magnetic field perturbation. Magnetic properties, e.g. magnetic moment, dia-magnetic and para-magnetic contribution of susceptibility for closed shell molecules have been studied.

5.1.2 Metallo-anti-aromaticity

Aromaticity in fully metallic systems has drawn very recent attention. It has been shown that Al_4Li_4 system behaves as anti-aromatic mixed metal systems. Al_4Na_4 and $Al_4Na_3^-$ were identified as another set of candidates for metallo-anti-aromatic system. Using electron localization function and density functional calculation, theoretical evidence of anti-aromaticity by showing electron transfer from Na/ Li to Al atoms was provided and the structures of these molecules were established. It was also shown that, for metallic systems, aromaticity or anti-aromaticity is primarily due to the sigma ring current and not just due to the electron counting rule of (4n+2) or 4n.



(a) (b)

(a) Al_4Na_4 and (b) $Al_4Na_3^-$ anti-aromatic structures

5.1.3 Complex scaled coupled-cluster technique

Complex scaling of the coordinates has been known as a technique to the calculation of resonance energies and the width. A highly correlated method has been considered to be essential for the purpose of accurate evaluation of these. The Fock space multi-reference coupled-cluster (FSMRCC) theory, with efficient incorporation of dynamic correlation and non-dynamic correlation arising due to near-degeneracy in the resonant states, has turned out to be the method of choice. Complex scaling in the FSMRCC method has been introduced to calculate shape and Auger resonance. This involves complex scaling of coordinates and subsequently solution of a complex Hartree-Fock equation, followed by the FSMRCC method, based on the complex orbitals. First numerical calculations of this method using the code developed have been presented for ^2P shape resonance of Mg and Auger $1s^1$ hole of Be.

5.1.4 Linear response to the Fock space multi-reference coupled-cluster method

In an important theoretical development, linear response formulation to the Fock space multi-reference coupled-cluster method has been developed. This is the state-of-the-art method for describing open shell systems and excited states. The linear response is based on a constrained variational functional for specific energy states within the Fock space framework, both for complete and incomplete model spaces and should obtain energy derivatives in an efficient manner.

5.1.5 Density functional response approach to molecular properties

Density functional method has emerged as an attractive alternative to more rigorous wave-function based methods for large systems, mainly because of its simplicity in retaining one-electron picture and yet its ability to include electron correlation. Fully analytic response approach of the density functional method to electric and magnetic fields is being developed for molecules. Thus molecular electric and magnetic properties will be obtained accurately within density functional approach. The Gaussian orbital basis set and an auxiliary basis to fit exchange-correlation part is used in the approach. The approach is being coded and soon the program system will be added to the popular package of density functional theory for energy and property, called deMON. The work has drawn attention of deMON developers, who have invited the work to be included in the package.

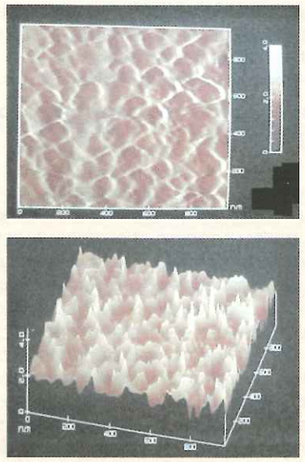
5.2 Materials chemistry & technology

5.2.1 Self-assembled monolayers for MEMS and monolayer protected clusters

Preserving the structural and functional integrity of interfaces and inhibiting deleterious chemical interactions are critical for realizing devices with nanoscale units. The presence of self-assembled monolayers (SAMs) on Si surface can tackle the stiction problem of micro-electromechanical systems (MEMS) by providing a suitable low energy surface coating. The antistiction properties of the monolayers can be tuned through suitable choice of chain length and terminal groups, for a number of applications such as molecular devices, lithography, and micromachines to inhibit Cu diffusion into SiO_2 in microelectronics devices. SAMs of difunctional molecules open up possibilities for preserving structural and

functional integrity of interfaces between nanoscale units of newly evolving device structures.

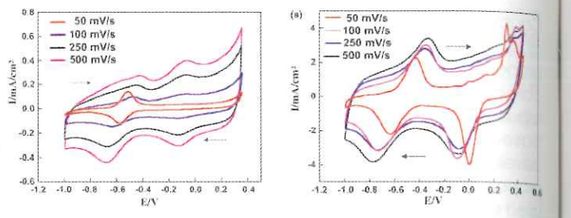
The objective is to make a self-assembled monolayer on Si substrate, which will act as an antistiction coating. A detailed understanding of the various aspects of the monolayer, such as ease of formation, adhesive properties, its stability, etc., need to be studied for device applications. An accurate control of monolayer growth kinetics is very crucial for closely packed and completely reproducible monolayers. Current work is focused on the adsorption kinetics and thermodynamic stability of octadecyl trichlorosilane (OTS) monolayers on Si. Initial studies showed the ability of OTS-SAM to control adhesion through surface functionalization. The photographs show the 2D (left) and 3D (right) AFM pictures of fully covered OTS monolayers on Si substrate, indicating a uniform growth mechanism.



5.2.2 Carbonaceous materials for ultracapacitors

Ultracapacitors are energy storage devices with potential application in electric vehicles. Specially designed materials with high surface area and ability for fast charge transfer are required to attain suitable powder density of these storage devices. Activated carbon and carbon nanotubes (CNT) have been identified as potential electrode materials for ultracapacitors. Highly conducting transition metal oxides attached on the carbon nanotubes are expected to give enhanced stability to them from degradation during sustained operation.

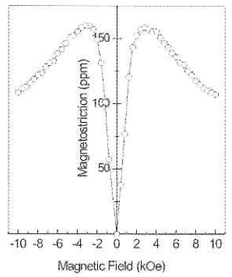
The work was focused on the statistical optimization of coconut shell carbon to get high surface area and capacitance. High surface area of 2300 m^2/g was obtained upon statistical optimization and separate samples give a capacitance of 150F/g. Preliminary experiments of CNT synthesis and the attachment of RuO_2 on multiwalled nanotubes (MWNT) has also been carried out. Functionalization of MWNT by ruthenium oxide caused enhanced capacitance of multiwalled carbon nanotubes from 30 F/g to 80 F/g. The following cyclic voltammetry graphs show the enhanced activity of the ruthenium oxide attached MWNT (right) when compared to that of the virgin nanotubes (left).



5.2.3 Development of oxide based magnetostrictive materials

Magnetostrictive materials are a class of smart materials with various technological applications. Magnetostrictive sensors and actuators are superior to other smart materials in terms of the non-contact operation and the possibility of absolute measurements. These materials are highly useful in different areas of strategic and technological importance. The currently used strategic magnetostrictive material, Terfenol-D, which is an alloy, suffers several drawbacks such as very high costs of terbium (Tb) and dysprosium (Dy), is extremely brittle, highly susceptible towards corrosion, magnetostriction is highly anisotropic, single crystals are required and therefore the high production cost of crystals, etc. Ceramic oxide based materials have the advantage of high chemical and thermal stability and the oxide ceramics are known for their high hardness and wear resistance, low coefficient of friction, low thermal conductance, low cost, easy processability, etc. It is possible to make the desired products of oxides into any shape by slip casting, dry press, extrusion, injection moulding, etc.

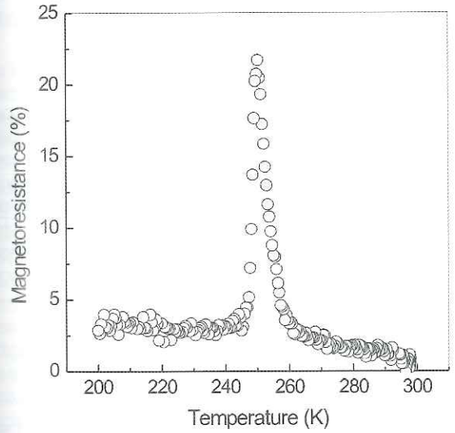
The work involves the development of suitable ceramic oxide magnetic materials, as a substitute for the currently available alloy based materials, for use as magnetostrictive smart materials. Different oxide magnetic materials such as cobalt ferrite, other ferrites, perovskite type oxides, etc. are being studied for identifying suitable materials. Relatively large magnetostriction at low magnetic fields, which is a prerequisite for many applications, is obtained for a cobalt ferrite based material, as shown in figure.



5.2.4 Studies on magnetoresistive oxides and similar systems

Perovskite type manganese oxides exhibiting magnetoresistive properties are fruitful candidates for future technological applications such as magnetic read/write heads, data storage etc. Huge changes in the magnetoresistance at very high magnetic fields and low temperatures are reported for this class of materials. For practical applications, however, sufficient magnetoresistance at relatively low magnetic fields and close to room temperature are highly desirable. The magnetic and electrical properties and processing-structure-property correlation of such systems to attain the above goals have been studied. Different types of perovskite type ferromagnetic materials are also being investigated to understand their phase diagram and the origin of their magnetic and electrical transport behavior as well as to look for new related ferromagnetic oxides, to resolve the problem of multiple magnetic phase behaviour etc.

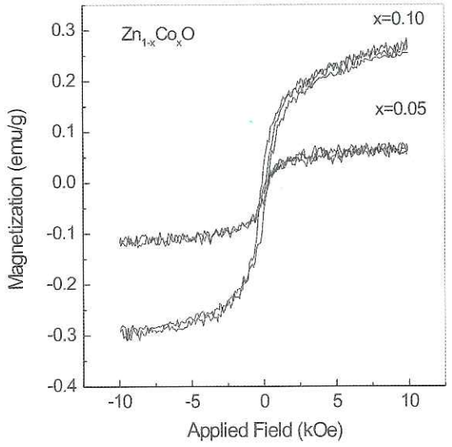
Above 20 per cent magnetoresistance at a relatively low magnetic field of 0.3 T was obtained for a calcium substituted polycrystalline perovskite manganate system, as shown below. Further emphasis is to obtain such properties at room temperature for various applications.



5.2.5 Development of oxide based diluted magnetic semiconductors

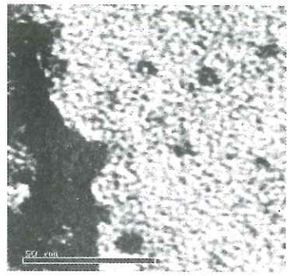
Diluted magnetic semiconductors are emerging new materials with many potential applications because of their semi-conducting as well as magnetic properties. These types of materials, based on simple semi-conducting oxides such as ZnO, are in the initial stages of development. Most of the studies are performed on thin films of the oxide. Ferromagnetism at or close to room temperature has been reported in ZnO, doped with small amounts of Co. However, for practical applications, it is desirable that the materials should be ferromagnetic much above room temperature. Similarly, ferromagnetic polycrystalline materials are useful for many device applications. Moreover, if the polycrystalline material can be produced as nanoparticles, this will be of particular importance for their use in ferrofluids, biomedical applications, magnetic recording, etc.

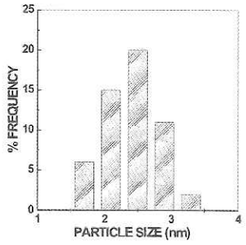
Emphasis has been on to synthesize these types of new materials by different synthetic routes, and especially to obtain polycrystalline materials, which are magnetic at or above room temperature. Ferromagnetism up to 770 K is observed, for the first time, in the nanocrystalline powders of ZnO doped with small concentrations of cobalt. Figure below shows the magnetization behaviour of two cobalt doped ZnO nanocrystallites at room temperature.



5.2.6 Nano-magnetic materials

Magnetic materials, in nanosized form, are useful for a variety of applications such as biomedical applications, magnetic storage, ferrofluids, etc. Currently synthesis and study of the magnetic properties of nanosized ferrite materials to optimize the processing conditions in order to obtain magnetic nanoparticles of small size, narrow size distribution, etc are being carried out. Various spinel type ferrites such as magnesium ferrite, nickel-zinc ferrite etc., which are being used for many technological applications in the bulk form, are currently under investigation. Apart from the synthesis of the ferrite nanoparticles for direct applications, sintering studies of these nanoferrites are also being carried out because low-temperature sintering is useful for enhancing the performance parameters of these ferrites for various applications as well as for lowering the production costs. Figure below shows nickel-zinc ferrite particles of 2.5 nm size and very narrow size distribution, obtained by a low-temperature method of synthesis.





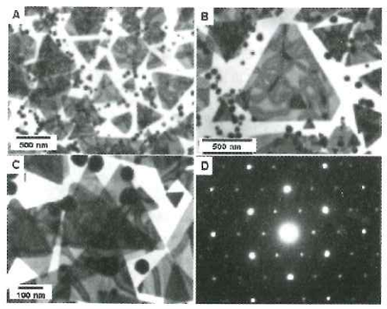
5.3 Nanoscience & technology

The primarily focus is on developing new methods for the synthesis and assembly of inorganic nanomaterials. Viewing nanomaterials as specialty chemicals, the focus is also on developing experimental methods for large-scale production of nanomaterials.

5.3.1 Biological methods for nanomaterials synthesis

The synthesis of metals, metal sulphide, minerals and oxide nanoparticles using eukaryotic organisms such as fungi has been demonstrated for the first time. The possibility of room temperature synthesis of oxides such as titania, zirconia and magnetite is an exciting one with significant commercial implications.

As an extension of this approach, the use of plant extracts in the synthesis of metal nanoparticles of variable shape has been demonstrated. Particularly exciting is the recent demonstration on the large-scale synthesis of triangular gold nanoparticles with plant extracts. These particles have unusual optical properties (large near infrared absorption) with potential application in hyperthermia of cancer cells and scanning probe microscopy



A-C. Representative TEM images of gold nanotrianglessynthesized biologically. D is a selected area diffraction pattern of the triangles showing that they are single crystalline and (111) oriented.

5.3.2 Nanoparticle growth in non-polar organic media

A new method has been developed for the single-step formation of metal nanoparticles of variable shape in non-polar organic solvents. This technique is applicable to a range of metals such as gold and Pt with important application in catalysis. Using Langmuir monolayers of molecules that are good reducing agents, a new strategy for the formation of nanosheets and nanoribbons has been developed.

5.3.3 Phase-pure core-shell nanoparticle structures

Nanostructures of the core-shell form have important applications in catalysis, biomedical applications. However, existing methods for their synthesis are complicated and do not yield phase-pure core-shell structures. A new method based on immobilizing reducing agents on the surface of nanoparticles has been developed to realize phase-pure structures. Keggin ions and amino acids have been identified as reducing agents that can be immoblized on nanoparticles and selectively 'switched on' to make core-shell nanoparticles.

5.3.4 Foam based method for synthesis of nanoparticles / minerals

With a view to develop a simple method for the large-scale synthesis of nanomaterials, a foam-based method has been developed. This is based on the large interfacial area populated by surfactant molecules in the foam that may be used to immobilize a range of metal ions (both anionic and cationic) and thereafter, chemically treated to produce metals, metal sulphides, oxides and minerals. Using the complex structure of the foams, nanoparticles with unusual morphologies have also been synthesized in foams.

5.3.5 Preparation of magnetic/ noble metal core-shell nanoparticles

Because nanoparticles of Co, Ni etc. are very reactive it was envisaged that giving them a protective coat with more stable metals like Au/Ag would not only improve their stability but also give us more manipulative ability as available for Au/Ag nanoparticles.

Co and Ni nanoparticles have been prepared by a novel foam based technique. They were converted to Co/Ni_{core}-Ag_{shell} by a simple transmetalation reaction. The mechanism responsible for the phase transfer of Ni nanoparticles capped with oleic acid in the presence of phosphoric acid is being probed. Other magnetic materials like Fe_2O_3, Fe are being prepared. Efforts are underway to prepare these nanoparticles on various solid supports like polyurethane, Al_2O_3 and activated carbon so as to study their catalytic applications.

5.4 Physical chemistry of solvation of ions

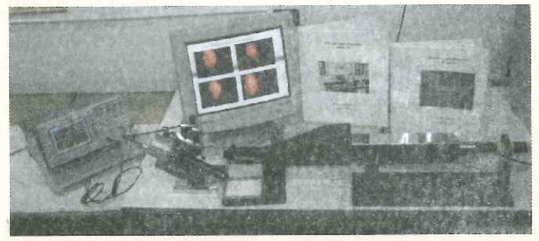
The viscosity dependence on the kinetics of bimolecular Cycloaddition reactions was examined. The enhanced reaction rates in low viscosity range were attributed to vibrational and translational modes in the solutions, while the rate declines in the higher viscosity range to diffusional barriers.

The concept of physical-organic chemistry was employed to transform the endo-selective cycloaddition to exo-selective one in the presence of ionic liquids. The ionic interactions responsible for achieving attenuation of hydrophobic effects caused by anti-hydrophobic agents were calculated from the experimental data on osmotic coefficients collected in the laboratory. These interactions and the departure of such systems from ideal behaviour were quantitatively estimated. The hydrodynamic behaviour of amino acids in aqueous ionic solutions was investigated in a variety of situations.

5.5 Instrumentation

5.5.1 Development of Brewster Angle microscope (Image 2K)

The instrument known as Brewster Angle Microscope (Image 2K), which is a PC based instrument, has been developed. This instrument is useful for imaging organic thin films and its morphology study. The instrument is import substitute and is useful for research in nanoscience area. This development has been completed with the sponsorship from Department of Atomic Energy. The technology includes p-polarized laser source, collimator, trough barrier assembly for monolayer compression driven by the intelligent microcontroller module, capturing and imaging system incorporating frame grabber card and CCD camera. The instrument has a facility of adjusting Brewster Angle for air-water interface and air-glass interface. The indigenous Image 2K software has been developed in VC++ environment having graphical user interface (GUI). Software features include real time imaging of monolayer at Brewster Angle, image analysis functions like brightness, contrast, domain area calculation along with file and print menu functions. The trough barrier movement is controlled by the intelligent microcontroller module, which receives commands, by PC through RS232 communication link.



In continuation with this development, another development has been initiated, which is Integration of Image 2K with LB trough using LabVIEW and Virtual instrumentation. LabVIEW VI will show both the image of the monolayer and the pressure area isotherm simultaneously. The development includes NI frame grabber and AD_DA card, interfaces, pressure sensor module etc.

5.5.2 Development of molecular beam instrument

Fabrication of Molecular Beam Instrument (MBI) and its implementation for catalysis research is an on going project. Along with fabrication of MBI, the development has been completed by ISG for the "Development of critical temperature controller" for heating the sample in Molecular Beam Instrument. The sample is to be heated up to 1200 ^{0}C by passing maximum current up to 30 amperes (DC) with low voltage. The instrumentation is developed to heat the sample in a controlled manner to required temperature. The temperature feedback is taken through K type thermocouple. The system is a close loop system. The sample temperature range is 200 to 1200^{0}C. The cooling of the system is manual. A ready-made and standard temperature controller cannot be used for this purpose.

6. Polymer science and engineering

6.1 Membrane science and technology

The work is being carried out on recovery of nonvolatile organic acids by perstraction and structure - permeation property relationship in polymeric membranes.

6.1.1 Recovery of nonvolatile organic acids by perstraction

Recovery of commercially important nonvolatile acids (citric, lactic, fumaric etc) produced by fermentation involves large number of steps and is also associated with waste disposal problem. Though membrane technology is an attractive alternative method as it reduces number of steps towards recovery of these acids, the demonstrated methods are based on electrodialysis or supported liquid membranes. These methods are tedious and may be cost intensive. Perstraction may provide simpler and cheaper process if adequate membranes are developed. The main objective of this program is to prepare and evaluate perstraction membranes that would have adequate flux and selectivity for nonvolatile acids over other organics.

The knowledge gained through previous work on TFC and UF membranes is applied to design new perstraction membranes for recovery of nonvolatile acids. On one side of the TFC membrane, a synthetic solution of lactic acid and other organics is passed, while other side is exposed to an extractant solution to withdraw the acid permeated through TFC. The prospective membrane materials are identified. The TFC membranes are being prepared and evaluated for permeation of lactic acid. The lactic acid is chosen as a representative of nonvolatile acids.

6.1.2 Structure - permeation property relationship in polymeric membranes

Gas permeation is a fast growing area of membrane technology. Various industrial gas separation processes are being successfully practiced. There is a wide scope to develop membranes for various applications with improved properties. Research in this field is directed towards invention of new polymeric materials that would combinely have (i) high permeability, (ii) adequate selectivity and (iii) processibility. Such materials will have high productivity in terms of flux as well as selectivity for desired component of a gas mixture and also will have capability to be processed in required membrane form such as hollow fiber or flat sheet.

The main objective of this program is to systematically explore polymer structures that would simultaneously have high permeability, selectivity and solubility in common solvents (to have easy processibility). Structural modifications through desired substitution on polymeric backbone belonging to different families of polymers, mainly polyarylates and polysulfones are being explored. The substitution on potential polymeric materials for gas permeation, such as polyphenylene oxide is also being done. The gas permeation properties and physical properties that are known to affect gas permeation are correlated with structural variations.Polyarylates and polysulfones using systematically substituted bisphenols and aromatic diacids, dense membrane preparation are synthesized and gas permeability and related physical properties are evaluated. Another potential candidate, PPO is being substituted with polar and bulky groups, which are anticipated to improve gas permeation properties.

6.2 Specialty polymers

6.2.1 Stimuli sensitive polymers for drug delivery systems

Polymer based excipients have been used in formulations for a variety of reasons, including taste masking, protection and stabilization of the drug, etc. The majority of prescribed drugs are designed for oral application since they have more patient compliance. However, patients at the extremes of age, such as children and the elderly, often experience difficulty in swallowing solid oral dosages forms. For these patients the drugs are mostly provided in liquid dosage forms such as solutions, emulsions and suspensions. The disagreeable taste of drugs causes difficulties in swallowing or causes patients to avoid their medication thereby resulting in low compliance of patients especially children are reluctant to take medicines on time. This creates problem in compliance to the dose regimens and poor results. The objective of this work was to synthesize stimuli sensitive polymers for the appropriate swelling and deswelling characteristic in the physiological pH media.

Novel polymers which can release the drug at the site of absorption without delay especially for the drugs with lower bioavailability and have specific region of absorption in GI Tract without alteration in dissolution and absorption were synthesized. Polymer characteristics which enable to maintain the drug in the substantially amorphous form and retain the same even during storage periods ensuring the rapid dissolution and hence the bioavailability of the drugs were evaluated. Synthesis and screening the polymers for their application in drug delivery based on their response to the different pH media, and the formulation of the dosage forms incorporating these polymers was carried out. The application of the polymer for the taste masking of bitter drugs in liquid oral preparation like dry syrups and suspensions and in tablets like dispersible and rapidly disintegrating and chewable was evaluated.

6.2.2 Supramolecular polymer synthesis

The supramolecular chemistry focuses on host guest interactions between two or more molecules that are not covalently linked. Crown ethers calixarenes, cyclodextrins and their derivatives have been commonly used to form complexes. These host guest complexes exhibit solution properties and reactivities different from those exhibited by the parent guest molecules. High rates of polymerization, higher molecular weights and ability to incorporate high loadings of hydrophobic monomers are some of the advantages offered by this technique. During the supramolecular complexes of hydrophilic and hydrophobic crosslinkers were prepared.

homopolymerization of complexed cross linkers by varying parameters such as initiator & chain transfer agent concentration was carried out. Copolymerization of complexed monomer with various hydrophobic and hydrophilic comonomers in various compositions depending upon the applications was undertaken. Light and heat curable acrylates polymers were synthesized and characterized.

6.2.3 Conducting polymers and their applications

The conducting polymers having extended pi conjugated electronic structure such as polypyrrole, polyaniline, polythiophene have been investigated for their applications in different electronic devices such as electrochromic displays, chemical / gas sensors, photo-electrochemical cells, electromechanical sensors and actuators. The bulk applications of these materials in EMI shielding, semi-conducting tapes for high voltage cables etc. have also been studied. To enhance the properties of these conducting polymers, modifications with functional groups, blending, incorporation of certain dopants, blending etc. has been carried out.

6.2.3.1 Functionalized conducting polymers and their applications

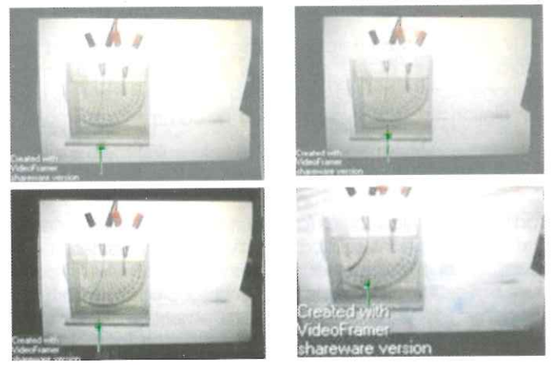
Chromatic effects in materials such as thermochromism, electrochromism, solvatochromism etc. have become important for many applications: as thermal indicators, sensors, display devices and so forth. Conducting polymers exhibit a number of these effects which can be further sensitized for enhanced colour ranges, contrast and fast response. Dye sensitization of conducting polymer has been studied extensively which has led to development of new materials having excellent properties for applications in optoelectronic devices.

Electrochromic effect in conducting polymers

These polymers after incorporation of functional dyes show large changes in optical spectra when exposed to organic solvent vapours, humidity etc. which can be effectively used for optical fiber based sensors having very fast response time.

6.2.3.2 Electroactive polymers for electromechanical actuators

Piezo-sensitive polymers are important materials for developing electromechanical devices: tactile sensors and actuators which have variety of applications in robotics, aero-space, biomedical devices and remote control systems. Conducting polymers are being studied for these applications. Large strains (bending) with application of small electric voltage (1 to 2 V) have been observed in these materials. The bi-layer actuator constructed using the conducting polymer with a backing insulating polymer film has been investigated for actuation response characteristics.



Conducting polypyrrole with PET backing layer as actuator. Arrows show original position at zero applied potential

6.2.3.3 Conducting polymers: Electro-catalytic processes

Conducting polymers possess charge transfer capability with redox type behaviour which can be effectively used for electro-catalysis. Their catalytic efficiency can be enhanced with certain doping agents. These materials have been demonstrated as excellent catalysts for Wacker type oxidation of alkenes, carbonylation reactions, electro-oxidation of methanol and reduction of nitrobenzene.

6.2.4 Polymers for UV/E-beam curable applications

Technology in coatings is resorting to UV and E-beam cured coatings to achieve environmental compliance and to improve customer satisfaction. UV curing formulations are the most rapidly growing technologies within coating, adhesives and related industries. On wood, plastic and paper, UV curing systems have been used to dramatically increase line speeds and to develop coatings having superior environmental resistance coupled with excellent gloss. The radiation curable protective coatings can be classified under (i) industrial coatings, (ii) powder coatings and (iii) resins targeted at graphic

arts industries. Industrial coatings apart from electronic industries are targeted at wood products, metal decoration and coating on plastics. Powder coating is suitable for highly automated product lines for product finishing such as metal appliances and automotive fittings. UV coatings in litho and offset serve graphic arts industry.

The objectives of the project are i) to develop synthetic strategy for synthesis of oligomer resins based on acrylated polyesters and to develop UV curable formulations using multifunctional oligomeric epoxy, urethane acrylates and establish curing characteristics and ii) to develop membrane bio-reactors with the use of UV curable formulations containing epoxy functionalities.

A UV curable commercial sample was obtained and the characterization of the sample is in progress. Some more urethane acrylates were synthesized and these samples after formulation would be evaluated with the commercial sample.

6.2.5 Functional polymers for chiral separations

Traditional chemical routes for drug synthesis result in a racemic mixture. The pharmaceutical activity generally resides in one enantiomer while the other may either be harmless or could have adverse health effects. In India chiral drugs are marketed in racemic forms. The current FDA requirement on chiral drugs is that only the active isomer ought to be sold. Considerable value addition results from the isolation of the active and desirable enantiomer. The objectives of the project were to develop commercially viable polymeric/ inorganic materials suitable for use as chromatography supports for high performance liquid chromatography and to establish scientific protocols through molecular modeling and simulation and to evaluate these materials for the efficient separation of optical isomers of racemic drug molecules.

Crosslinked polymers with varying crosslink densities were synthesized as a continuing exercise. The polymer matrices were sent to RRL, Jammu and IICT, Hyderabad. Some of the polymer matrices were tested in-house for immobilization on Lipase. Some of these samples showed good immobilization characteristics. Esters of Ibuprofen were prepared and the evaluation is in progress. From the polymer matrices samples sent to RRL, Jammu, three polymers showed good binding to Y15, RRL1 and RL1789. Preliminary evaluation indicated that the immobilized enzymes were suitable for the resolution of drug intermediates.

6.2.6 Novel hydrophobically modified polymers: synthesis, characterization and rheology

Synthetic water-soluble polymers are being extensively developed and used as viscosity modifiers in various water-based fluids. However, conventional water-soluble polymers suffer from drawbacks in which their solutions are unstable towards shear, temperature, pH and the presence of salts.In order to overcome these drawbacks, the concept of associative polymers with reversible association was introduced and consequently, hydrophobically modified polymers [HMPs] have emerged as an excellent materials because of their unusual rheological properties. These polymers consist of a water-soluble hydrophilic backbone and a small amount (~typically < 2-5 mol %) of covalently bound hydrophobic moieties called 'stickers'. The molecular architecture as well as the characteristics of the hydrophilic chain and the stickers can vary widely and give synergistic effects. Therefore, the architectural richness of HMPs (random, block or hydrophobically end-capped) gives diverse physico-chemical properties, which have applications in cosmetics, paints, textile pastes, papers, drilling fluids, detergents and pharmaceuticals.

Designing and synthesizing new hydrophobic compounds from cashew nut shell liquid and gallic acid and development of novel HMPs using these hydrophobic compounds is being carried out. These HMPs have shown superior properties compared to their unmodified precursors and have potential applications in cosmetics and pharmaceuticals.

6.2.7 Design and synthesis of new thermoreversible LCST hydrogels.

Thermoreversible polymeric hydrogels exhibit the thermodynamic lower critical solution temperature (LCST) and undergo swelling-shrinking (collapse) first order volume transitions at LCST. For example, poly(N-isopropyl acrylamide) [PNIPAm] and poly(vinyl methyl ether) [PVME] gels possess the LCSTs of 32°C and 38°C, respectively. Below these temperatures, the gels swell in the solvent and shrink above this temperature expelling most of the solvent absorbed. Hence, they are also termed as "Thermoshrinking" polymers. The property of temperature dependent swelling-shrinking of thermoreversible gels has made them as promising materials in the areas of controlled drug delivery, bioseparations, biomedical fields, etc.

Interactions between polymers and surfactants play an important role in determining conformation transitions, phase separations, volume transitions and rheological behaviour of polymer solutions. In this project the interaction between anionic surfactant, sodium dodecyl sulfate (SDS) and copolymer gels namely, PNIPAm-co-poly (amino acids) has been investigated. Core-shell morphology in the swollen gels along with two discontinuous volume transitions has been observed. Such morphologies have potential applications in drug delivery systems. A mechanistic interpretation of these new observations on the basis of electrostatic charge repulsion and restricted diffusion of surfactant into the gel was also provided.

RESEARCH & DEVELOPMENT REPORTS
POLYMER SCIENCE AND ENGINEERING

6.3 Polymer degradation & stabilization/ environment friendly polymers

6.3.1 Studies in polymer degradation

SEPAP 12/24 photoirradiation chamber

Accelerated thermal ageing oven

The polymeric materials constitute one of the fastest moving frontiers of the polymer science but most of them undergo more or less rapid degradation upon exposure to the natural and induced environmental conditions due to combined action of the solar radiation, atmospheric oxygen, humidity and temperature. To improve all aspects of the stability of polymers, a fundamental and complete understanding of the degradation process involved is essential to control the destructive reactions.

Generally conventional stabilizers are low molecular weight compounds, therefore, may leach out/ volatilize/ migrate from the polymer surface. The surface grafting/ anchoring of stabilizer is a convenient technique to effectively protect/ to increase the service-life of the polymers against photodegradation. A polymeric HALS which offered the right balance of diffusivity and compatibility of the stabilizer in the polymers has been synthesized. UV absorber (benzotriazole) and/ or HALS moieties to the anthraquinone dyes were attached to check the photofading of dyed nylon 66. other hand, to the performance of materials and products.

6.3.2 Eco-friendly and bio-degradable polymers

The aim of this project is to synthesize polymers based on reaction of sugar molecules with polyolefins, with a view to converting the material to a nutrient source for microorganisms, with a view to making them useful as biodegradable polymers. Work is being carried out on development of new series of biodegradable polymers based on attaching glucose, sucrose and lactose onto synthetic polymers in minute quantities in order to introduce the properties of biodegradability in these non-biodegradable polymers.

6.4 High performance polymers

High performance polymers such as aromatic polyesters, polyimides, polyamides, polyethersulfones and polyetheretherketones, represent important commercial materials. Many high technology applications in the areas of aviation, electronics, etc., rely on high performance polymers as key constituents. Much of the focus in the area of high performance polymers is on tailoring polymer structure to give a specific set of properties.

The main objective of the work was to design and synthesize novel difunctional monomers, viz., bisphenols, diamines, and diacids having special structural features, such as flexible linkages or rigid moieties, which when incorporated into high performance polymers would impart unique property combination to them.

A series of new bisphenols containing rigid moieties were synthesized starting from commercially available inexpensive chemicals, such as, biphenyl, naphthalene and 2-naphthol by a series of simple organic reactions. The bisphenols were utilized to synthesize a host of high performance polymers such as aromatic polyesters, polyimides, polyamides, polyether sulfones and polyetheretherketones. Incorporation of these monomers into high performance polymers resulted into polymers with improved thermal properties and at the same time with improved solubility in common organic solvents. Thus these polymers can be considered as promising class of processable high performance polymers. These polymers are under evaluation as membrane materials for gas separation.

Another promising approach that was looked into was to obtain monomers containing pendant C15 alkyl chain starting from cashew nut shell liquid (CNSL) a renewable resource material. Starting from CNSL, a series of novel monomers, viz., diamine, diacid, and bisphenol were synthesized. Work is under progress to synthesize high performance polymers based on the above monomers.

6.5 Complex fluids & polymer engineering

The central theme is to understand the links between the microstructure of complex fluids and their fluid and solid-state properties. These links are related on the one hand, to the kinetics and thermodynamics of structure formation and, on the other hand, to the performance of materials and products.

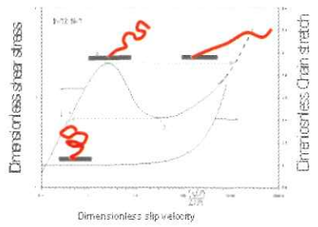
The State-of-the-art rheometers: an ARES (controlled strain rheometer), a BOHLIN CVO-50 (controlled stress rheometer) and a RHEOVIS 2100 (high shear capillary rheometer) allow for measurement of all material functions of complex fluids under shear flow. Rheo-optical techniques to study stress-birefringence in viscometric and complex flow fields are being developed. The capability to do POLYFLOW viscoelastic CFD simulations to match rheo-optical data and perform extrusion simulations is also being built. The lab has facilities useful for wet chemistry such as fume hoods, vacuum ovens, rotovap, centrifuges, etc. Pilot scale polymer processing and mechanical testing facilities in the Polymer Processing Center (PPC) such as the DSM microcompounder and microinjector, Berstorff ZE-25 twin-screw extruder, Haake Polylab system, Arburg injection molding machine, Instron UTM and Ceast Izod impact tester are also used.

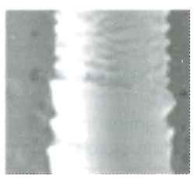
ARES

Bohlin CVO50

6.5.1 Stick-slip phenomena in polymers

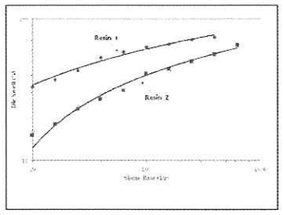
Wall-slip is a phenomenon that limits the productivity of melt-extrusion processes for highly entangled polymers such as polyethylene. The stick-slip transition above a critical wall shear stress in extrusion was modeled by developing a constitutive equation using tube (repetition) theories to describe the coupled dynamics of bulk chains and of the strongly adsorbed end-tethered chains under various regimes of wall grafting density. As shown in the figure, the molecular origin of the stick-slip instability is related to a sudden stretching of tethered chains and their consequent disentangling from bulk chains above a critical stress.

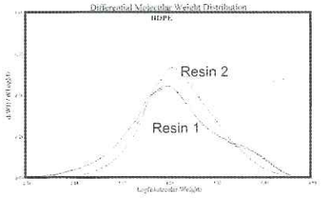




6.5.2 Fingerprinting of commercial polymers

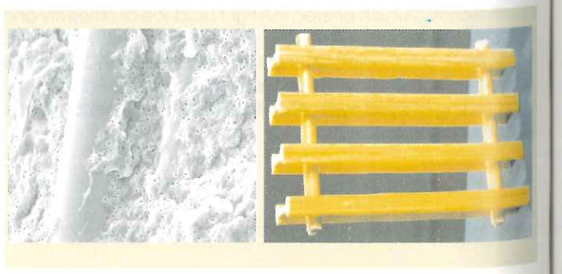
Research was undertaken to understand the structure-property relationships in resins and the scientific reasons for better performance of leading resins in the markets. The figure shows how the die swell of two blow molding resins is intimately linked to their MWD. The resin with lower polydispersity exhibits higher transient die swell due to rapid relaxation.





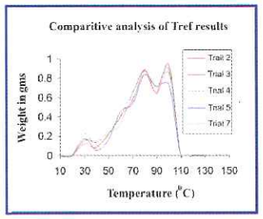
6.5.3 New product development

PP-glass composite compound having a targeted set of mechanical properties has been developed. The figure shows the 3-phase morphology of the PP-composite in which the glass fibers have excellent adhesion to the matrix and the matrix itself consists of uniformly dispersed fine domains of a polyamide. Several polyester-glass pultruded profiles were developed using the pilot-scale PULTREX pultrusion facility in the PPC. These include C-, I-, rod, and notched section profiles for applications in gratings and ladders.



6.5.4 Development of new equipment

A preparative temperature rising elution fractionation equipment was designed and built. Reproducibility of the eluted weight fractions of a ZN-LLDPE resin obtained from programmed heating steps after a slow cooling cycle is shown in the figure.

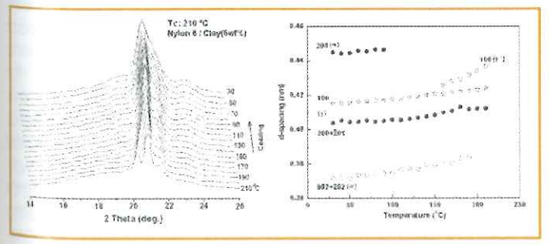


6.6 Polymer nanocomposites

6.6.1 Nylon - clay nanocomposites

The nanocomposites were prepared by melt mixing nylon with desired amount of clay in DSM Micro Twin Screw Compounder at 230 °C for 5 min (100 rpm). The X-ray diffraction experiments were performed using Rigaku Dmax 2500 diffractometer with a high temperature sample stage. Thermogravimetric analysis was used to determine amount of clay present in the nanocomposites.

The new peak at 2θ = 20.327° indicates presence of an additional phase and its position is more close to the 200 reflection of the phase and is called the metastable phase. The metastable phase transformed into γ-phase on cooling at about 150°C and the transformation is reversible on heating.



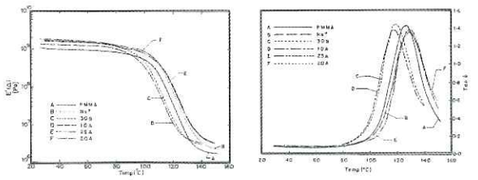
X-ray diffraction patterns and change in d-spacing on cooling to room temperature from crystallization temperature 210°C

6.6.2 Poly (methyl methacrylate) (PMMA) based nanocomposites

PMMA-clay nanocomposites prepared using organically modified layered silicates are being studied. These materials were prepared using the melt mixing route on small (50g) as well as industrial (700 g-1 kg) scale, for evaluation of various thermal and mechanical properties. The PMMA -Montmorillonite hybrids were characterized by WAXD, TGA, DSC, tensile deformation and dynamic mechanical analysis. Except for the hybrid formed with unmodified sodium montmorillonite where a change in distribution of clay platelet stacks was observed without polymer intercalation, use of organically modified montmorillonites gave well intercalated systems. Increase in the clay layers separation, due to polymer intercalation, was observed in the range 7-14 Å. TGA thermographs indicate that the onset of decomposition increased by 15-30 °C, depending on the organoclay, as compared to PMMA itself. DSC results show the existence of a glass transition temperature (T_g) for all the hybrids and that the T_g of the hybrids are less (by ~10%) compared to that of PMMA. Among the various modifiers, the ones that are relatively more polar favor a greater extent of intercalation of PMMA into the clay layers. The thermal stability of the nanocomposite is superior to that of PMMA, and is controlled by the stability of the organoclay and its interaction with PMMA.

Organic modifiers used in the study and TEM micrografs of intercalated PMMA nanocomposites.

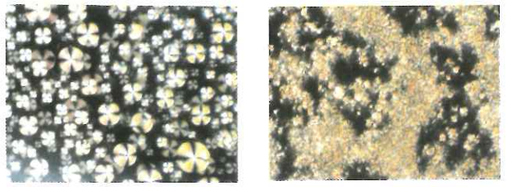
A significant improvement in the Young's modulus of the nanocomposites is seen compared to that for unfilled PMMA. The unintercalated composite formed with pristine clay showed smaller enhancement in the tensile modulus compared to intercalated nanocomposites based on organically modified clays. The use of organoclays that contain polar groups on the exchangeable quaternary amine results in a relatively smaller increase in the modulus as compared to when more hydrophobic (not containing polar groups) organoclays are used. The elastic modulus in the solid state below the glass transition temperature is higher for the intercalated nanocomposites as compared to unfilled PMMA with minor differences as affected by the organic quaternary amine treatment of the clays.



Storage and loss moduli of intercalated PMMA nanocomposites by dynamic mechanical analysis

6.6.3 Liquid crystalline polymer nanocomposites

Work on intercalated nanocomposites of poly(ethylene terephthalate-co-oxybenzoate) [PETOB] and layered aluminosilicates (montmorillonite clays) is focused towards the effect of organoclay and its loading on liquid crystalline phase behavior and nano-meso scale structure. The study is being carried out in significant depth in order to understand how these advanced materials behave as controlled by molecular parameters. Characterization of the morphology of intercalated nanocomposites of PETOB, at 2% by wt. clay loaded into this thermotropic liquid crystalline polymer matrix, shows existence of the nematic phase in the temperature window 190°-220° C. Various organoclays have been studied in this work. The nematic phase optical micrografs for intercalated nanocomposites prepared with organoclays having different chemical structures of the organic modifier, show existence of liquid crystallinity for all nanocomposites. TEM imaging performed on ultrathin microtomed specimens show a homogeneous dispersion of clay platelet stacks throughout the polymer matrix.

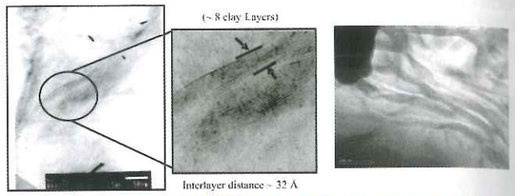


Optical micrografs of liquid crystalline phase of PETOB copolyester and its nanocomposites with clay

In addition, a somewhat spatially oriented dispersion of clay stacks is also observed in few regions of the hybrids. Scenarios such as partial intercalation of polymer in-between successive clay layers due to processing during hybrid preparation are also seen. Intercalated clay platelet structure is clearly observed at high magnifications indicating favorable nanoscale thermodynamic interactions between the polymer chains and the clay surface. This has also been confirmed by X-ray diffraction measurements. Oriented clay stacks are rationalized to occur due to stack-stack interlayer energetic interactions in presence of crystalline polymer phase at room temperature.

TEM micrografs of various regions of intercalated PETOB-clay nanocomposites

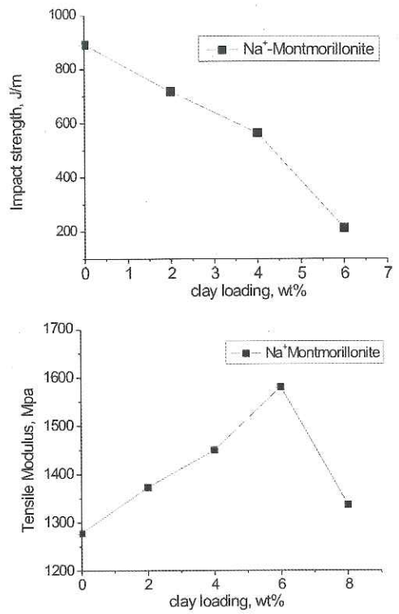
In general, in most regions of the nanocomposites, the nearest neighbor clay stacks exhibit random orientational order over smaller as well as larger distances. The formation and observations in case of nanocomposites prepared with organically modified montmorillonites, showed that favorable thermodynamic interactions exist between the clays and the polymer segments, resulting in intercalation of polymer chains while maintaining liquid crystalline behavior of the overall polymer matrix.



Nanoscale structure of PETOB intercalated nanocomposites as studied by TEM

6.6.4 POM homopolymer and POM-PEO copolymer nanocomposites

New intercalated and novel partially exfoliated nanocomposites of Poly(oxymethylene) {POM, Acetal resin} were prepared using sodium montmorillonite (MMT), organomontmorillonite and laponite clays, by the melt processing route. Processing conditions such as batch mixing speed, time and temperature were varied and optimized in order to obtain stable nanocomposites under most desired operating conditions. POM intercalates into Na^+MMT to separate the clay layers by 7 Å. Specific organic modification to montmorillonite rendered the silicate sufficiently organophilic but maintaining the polar interactions between POM chains and organic modifier surfactant, thereby leading to significant levels on intercalation (effect d-spacing shifts approx. 20 Å and 7 Å, respectively, for the organoclays studied). Partial exfoliation was also observed in the case of nanocomposites formed using dioctadecyl diethoxy quaternary ammonium exchanged montmorillonite. POM nanocomposite was fully exfoliated when nanometer sized clay laponite was employed. Melting temperatures (T_m) of the nanocomposites are comparable to that of crystalline POM and remain unaffected as a function of clay type and size. Significant increase in crystallization temperature as compared to unfilled POM is observed by formation of nanocomposites for all clays. Enthalpy of melting is significantly higher for the nanocomposites as compared to POM. The nanocomposites are thermally more stable as seen from TGA (weight loss on heating) results. Tensile and impact properties were also studied using injection molded specimens via DSM microcompounder. Higher tensile modulus for nanocomposites as compared to POM is observed, the modulus increasing with clay wt%. Impact strength is lower for the nanocomposites and decreases with increasing clay loading. Comparison of results for POM nanocomposites with preliminary results on intercalated nanocomposites of coacetal resin {Poly(oxymethylene-co-ethylene oxide)} are also being carried out. Preliminary results on the nanocomposites of POM-PEO with the organoclays showed intercalated structure.



Variation of impact strength and tensile modulus of POM nanocomposites

6.6.5 ABS and SAN nanocomposites

Several new intercalated and exfoliated nanocomposites of acrylonitrile-butadiene-styrene (ABS) resin with layered silicates were obtained by melt state processing route. The effects of organic modifier structure of the clay in case of montmorillonites (MMT) and also at the effect of clay layer size by utilizing laponite clay were studied. The nanocomposites were characterized using X-ray diffraction, DSC and TGA. The effect of clay weight loading on the nanocomposite d-spacings and its thermal stability and properties were investigated. The tensile modulus of the nanocomposites are superior to that of the unfilled polymer by 4% - 30% depending on the type of clay, at similar and low loadings such as just 4% by wt. clay in the hybrid. d-Spacings of the hybrids by the batch mixer route, are not affected by using rotor speeds higher than 60 rpm. There is significant increase in several mechanical properties such as stress at auto-break, modulus, tensile strength by the formation of intercalated nanocomposites, while strain at auto-break significantly decreases due to the presence of intercalated clay. At low and reasonable loadings, the yield stress of the intercalated nanocomposite prepared using organically modified montmorillonites are higher than that of ABS, while yield stress of ABS-Na^+MMT composite is not much different from that of ABS. Both notched as well as unnotched impact strengths of the nanocomposites are inferior to that of ABS, except in two nanocomposites where an increase in the impact has been observed. Use of 30nm sized laponite clay leads to exfoliated nanocomposites and an improvement in impact strength (ductility) compared to the polymer. Results using different processing equipments such as Brabender batch mixer (50 g scale), large scale twin-screw extruder (700 g scale), and DSM twin-screw extruder/ compounder (5g scale) are being completed.

6.6.6 HIPS and PS nanocomposites

Several intercalated nanocomposites of Polystyrene (PS) and high-impact polystyrene (HIPS) with layered organosilicates were prepared by melt processing methods and characterized for their nanoscale structure, thermal properties and mechanical properties. Organically modified clays, having different modifier chemical structures, are utilized in this study in order to look at the effects of physical chemistry on the nanoscale intercalation and thermal properties of the hybrids. The mixing preparation conditions such as rotor speed (rpm) and time of mixing were varied and optimized for preparing well intercalated nanocomposites with significant d-spacing changes accompanying nanocomposite formation. The nanocomposites are characterized using X-ray diffraction, differential scanning calorimetry (DSC), thermogravimetric analysis (TGA) and transmission electron microscopy. The effect of organic modifier on the clay surface (physical chemistry of clay) was also studied. The effect of clay loading into HIPS matrix is also investigated in the weight range 2-12 %. Well intercalated nanocomposites are formed for all clay systems and at all loadings investigated here. Intercalation and filler presence gives rise to enhanced tensile properties. Use of high hydrophobic coverage (dioctadecylammonium quat. based) organoclays does not give intercalation. The weight loading of clay into the polymer matrix is varied in the range 3-6%. HIPS intercalates to a slightly greater extent as compared to PS into the clay interlayer space, other conditions remaining the same, for the loadings and organoclays studied. Higher rotor speeds (rpm) leads to greater intercalation for all systems, however equilibrating at about 60 rpm. An increase in the clay loading leads to a decrease in interlayer d-spacings in the nanocomposites. For HIPS as well as PS nanocomposites, the T_g of the nanocomposites, studied by differential scanning calorimetry (DSC), shows a slight decrease compared to unfilled polymer, the effect being more in the case of HIPS relative to PS. Optimum mixing speed and time of mixing has been established for preparation of the hybrids. The glass transition temperature of the nanocomposites are similar to or slightly lower than those of HIPS in low clay loading range (<6% by wt clay). Comparison is made in certain cases with the behavior of polystyrene (PS) nanocomposites (intercalated) for the dispersion structure and level of polymer intercalation into the clay interlayer spacings, using the same clays. Results for a clay loading range till 12% by wt.are completed, using a variety of different organically-modified montmorillonites.

Polystyrene (PS)			High Impact Polystyrene (HIPS)		
System	Clay loading (wt.%)	T_0^* (°C)	System	Clay loading (wt.%)	T_0^* (°C)
PS	Zero	450	HIPS	Zero	460
PS-6A	3	470	HIPS-6A	3	470
PS-6A	6	460	HIPS-6A	6	465
PS-15A	3	480	HIPS-15A	3	480
PS-15A	6	460	HIPS-15A	6	480
PS-20A	3	475	HIPS-20A	3	480
PS-20A	6	465	HIPS-20A	6	480

Thermal degradation properties of intercalated PS and HIPS nanocomposites

6.6.7 PPO nanocomposites

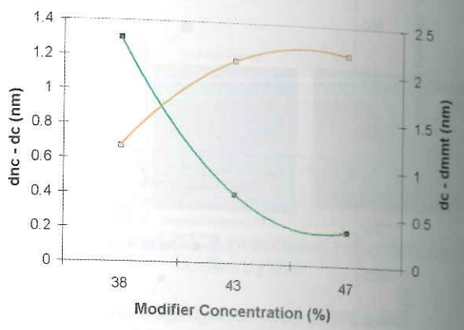
Study on preparation and characterization of layered silicate filler based nanocomposite materials using poly(phenylene oxide) {PPO} is being carried out. PPO is of significant interest commercially as well as from fundamental scientific research perspective. Intercalated nanocomposites were prepared by melt state processing method using different organically modified montmorillonite clays. Structural characterization of interlayer d-spacings using wide and small angle X-ray diffraction showed significant amount of penetration of PPO chains in between the silicate layers. The objectives of this study are to understand the influence of molecular parameters and process variables on structure and chain dynamics in these nanocomposites and to understand the influence of clays on a well studied classical fully miscible molecular blend. In order to understand the behavior of blends based nanocomposites, the nanocomposites of the individual polymer phases are also being carried out for comparison.

6.6.8 Effect of molecular size and molecular structure of the intercalant on structure and viscoelastic properties of nanocomposites

The cation exchange capacity of the layered silicate along with the molecular size and molecular structure of the organic intercalant controls the degree of intercalation of the polymer in the layered silicate. The concentration of the intercalant molecule as well as its size, thermodynamically govern the number of polymer chains infiltrating the silicate layers. The adjoining figure shows that as the concentration of the intercalant molecule increases the amount of polymer chains infiltrating the silicate gallery decreases.

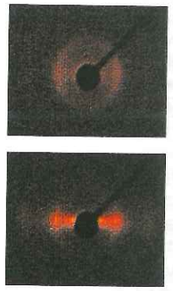
The amount of polymer chains infiltrating the silicate gallery governs the viscoelastic properties of the PLS nanocomposite. The amount of polymer intercalated in the silicate gallery space is more for layered silicates having small intercalant molecules. Also the presence of specific interactions between the functionalities in the intercalant molecule and those in the polymer also increases the amount of polymer intercalated.

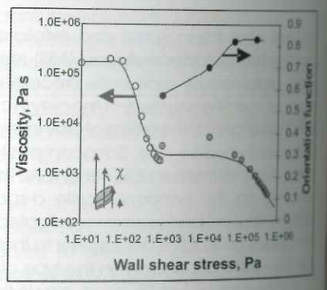
These nanocomposites having higher amount of polymer present in the silicate gallery showed better mechanical properties than those in which the amount of polymer intercalated was less.



6.6.9 Rheology of nanocomposites

The rheology of polymer nanoclay composites is extremely sensitive to the clay dispersion, loading and orientation. Polymer layered-silicate nanocomposite melts exhibit visco-plastic rheology with an apparent yield stress below which the melt consists of a percolating network of clay tactoids and above which these tactoids rapidly orient along the flow direction. The figure shows the flow alignment of clay tactoids with increasing shear stress as captured by in-situ rheo-XRD measurements using the Cambridge MultiPass Rheometer.





6.7 Structure - property relationships in polymers

Morphology, the science of form and structure, provides the link between the molecular structure and the bulk properties. As applied to polymers, morphology involves the study of the arrangement of polymer molecules into crystalline and amorphous regions. The semi-crystalline polymer properties are directly linked to the structure and morphology. Nylons are the one among the most successful semi-crystalline polymers and nylon 6 is the key member of the nylon family. Similarly syndiotactic polystyrene (sPS) is the newly developed semi-crystalline polymer with high melting point and exhibit excellent mechanical and solvent resistant properties.

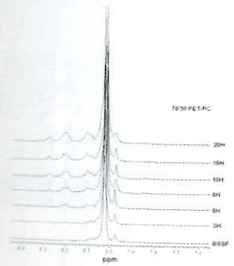
The objectives of this study are: i) *in-situ* high temperature Fourier transform Infrared spectroscopic (HT FTIR) studies on the clathrate form of syndiotactic polystyrene (sPS) during heating and ii) to study the crystallization behavior of Nylon 6 in the presence of layered silicates.

6.7.1 Morphological consequences of interchange reactions during solid state copolymerization in poly (ethylene terephthalate) and polycarbonate oligomers

Poly(ethylene terephthalate) (PET) is the most prominent member of thermoplastic polyester family. Some PET applications require modification of the base polymer. For example, in blow molding an increase in the glass transition temperature is useful in reducing the crystallization ability and increasing the melt strength. Also, it is less tough and soluble in more aggressive solvents such as trifluoroacetic acid (TFA) and o-chlorophenol. Bisphenol A polycarbonate has high impact strength and is soluble in common solvents such as chloroform. A copolymer or a blend made from the two could give a new material with combined properties.

The purpose of this study was to examine the development of structure and morphology during ester-carbonate interchange reaction and solid state polymerization of PET/PC oligomer blend. The PET/PC oligomers were initially melt blended and crystallized. The crystallized blend was subjected to simultaneous solid state polymerization and ester-carbonate interchange reaction by holding the blend just below the melting temperature under reduced pressure. The change in the structure and morphology was monitored by 1H NMR spectroscopy, DSC and X-ray diffraction.

Poly(ethylene terephthalate-co-bisphenol A carbonate) was successfully obtained by simultaneous solid state polymerization and transesterification of crystallized PET/PC oligomers. The transesterification and degree of randomness increases simultaneously with SSP. According to Bernoulli's statistics, degree of randomness values indicates that the polymer obtained during SSP is a block copolymer. The DSC and WAXS results revealed the amorphization of PET and PC crystals below the melting temperature with the progress of SSP and transesterification.

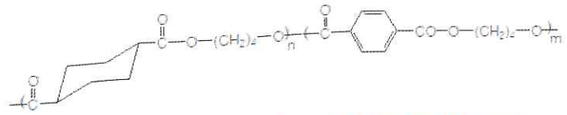


The appearance of new peaks at 8.14, 8.20 and 8.30 ppm indicating the exchange reaction between PET and PC oligomers simultaneously with chain extension

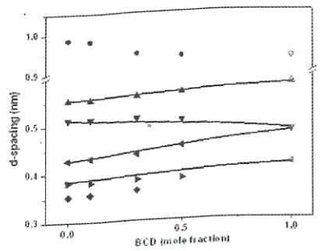
6.7.2 Structure-property studies in aliphatic aromatic polyesters

Aliphatic aromatic polyesters are a class of thermoplastic polyesters with useful properties like high heat distortion temperature, high rigidity, good mechanical properties, toughness, excellent surface appearance, good chemical resistance and stable electrical-insulation properties. The commercially successful polymers of this class are the poly(ethylene terephthalate), poly(butylene terephthalate) and poly (ethylene naphthalate)s. Among these polymers, PBT is a fast crystallizing polymer and, hence, well suited for extrusion and injection molding applications. However, at T_g (~ 40C) the mobility of the polymer chains in the amorphous regions increases considerably, resulting in decrease in stiffness. Hence PBT is not suitable for applications involving high heat. The properties of PBT can be modified in many ways to meet the requirements of specific fields of application. Copolymerization, blending with other polymers and addition of additives are different ways to modify the properties of PBT. Cycloaliphatic diols impart molecular rigidity to the polyester chain.

A series of poly(butylene terephthalate-co-1,4-cyclohexylene dimethylene terephthalate)s (P(BT-co-CT)) and poly(butylene terephthalate-co-1,4-cyclohexane dicarboxylate)s (P(BT-co-BCD)) copolymers with various CT and BCD contents were synthesized by melt polycondensation. The poly(BT-co-CT) copolymers exhibited typical eutectic behavior in melting and crystallization with a eutectic composition corresponding to $PBT_{75}CT_{25}$ indicating iso-dimorphic cocrystallization behavior. On the other hand, poly(BT-co-BCD) copolyesters showed isomorphic crystallization but did not show eutectic behavior in melting and crystallization. The glass transition temperature showed linear dependency on composition in these copolymers.

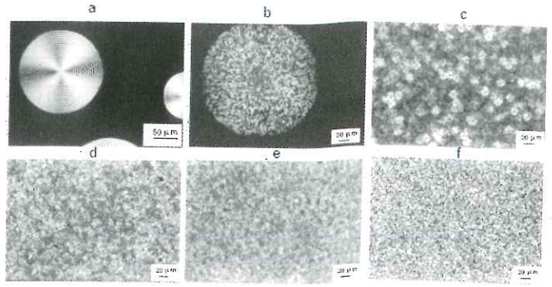


Poly(butylene terephthalate-co-butylene cyclohexane dicarboxylate) (poly(BT-co-BCD))



Changes of d-spacings for poly (BT-co-BCD) copolymers with copolymer composition (,) 001(along chain direction), (7) $0\bar{1}_1$, (B)010, $(\Omega)\bar{1}_11(\beta)100$ and (Λ) reflections (based on PBT structure) as a function of copolymer composition

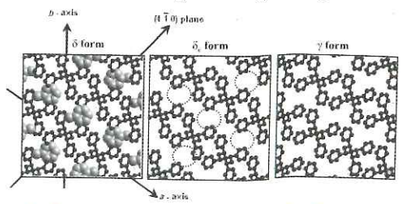
The spherulitic morphology of the copolymer depends on the composition of the constituent polymers. In the case of poly(BT-co-CPDT) copolyesters, the polarizing optical microscopy studies showed gradual change in the morphology of the spherulites with increase in PBT content.



Polarized light micrographs of (a) PCPDT (b) $PBT_{15}CPDT_{85}$ (c) $PBT_{45}CPDT_{55}$ (d) $PBT_{78}CPDT_{22}$ (e) $PBT_{85}CPDT_{15}$ (f) PBT

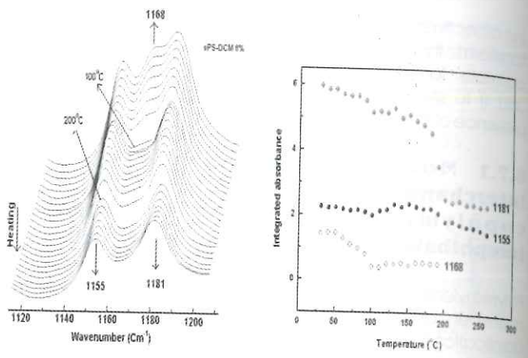
6.7.3 Polymorphism in syndiotactic spolystyrene

Amorphous syndiotactic polystyrene (sPS) films were crystallized in the clathrate form by immersing in DCM, Toluene, DCB, Decalin, and Acetone. IR spectra were taken using Perkin-Elmer FTIR Spectrometer (model PC 16) at 2 cm^{-1} resolution, in the range 450 - 4400 cm^{-1} and 32 scans for signal averaging. High temperature spectra were obtained by mounting sample in Mettler Toledo FP82HT hot stage and placing it in the sample compartment of FTIR and aligned using laser light.



Interaction between polymer and solvent along the b axis, is different while along the a axis is almost common for all the helical forms

The FTIR spectra showed major changes when γ form transformed into α" form at ~200°C, when the helical conformation changes into planar zigzag conformation. On the other hand, the transition of δ form into γ form on heating above the glass transition temperature is not very obvious, as the spectral changes are only marginal and affects very weak bands.



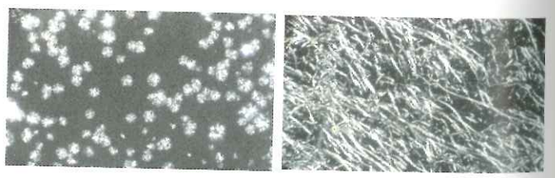
The 1168 cm^{-1} long helix band assigned to TTGG conformation responds to δ to γ form transition. It is dependent on amount of solvent in the clathrate

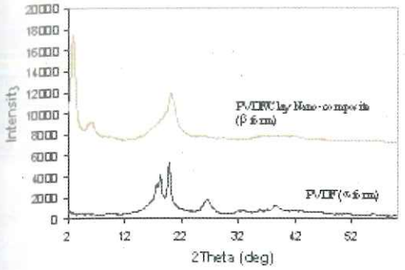
6.7.4 Crystallization of polypropylene

Polypropylene (PP) is known to exhibit well-defined spherulitic morphology when crystallized from melt at 122°C. In the nanocomposite, however, the crystallization of PP takes place even at a higher temperature of 142°C and the crystallites grow as fibers that increase in diameter. This indicates that the surface of the exfoliated layered silicate acts as a nucleating agent that promotes crystallization of PP. The figures show the optical micrographs for PP and PP/clay nanocomposites crystallized at 122 and 142°C, respectively.

6.7.5 β Phase in polyvinylidenefluoride

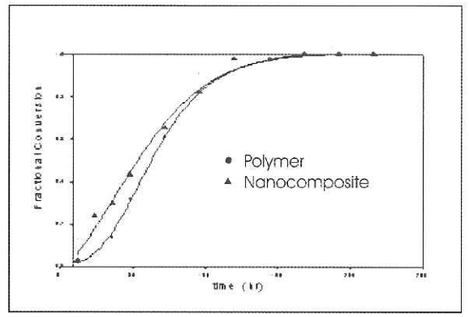
Phase in polyvinylidenefluoride (PVDF) exhibits polymorphism and is known to crystallize in four different forms namely α ,β , γ, and δ . The most readily formed crystal structure is the α form and can be obtained by cooling from the melt. On orientation it converted to the β form, which is of great importance because of its piezo- electric effects. A stable β phase in PVDF was obtained from intercalated PVDF/clay nanocomposites, which was confirmed by annealing the sample above the melting point. The figure shows WAXD pattern confirming the formation of β form of PVDF.

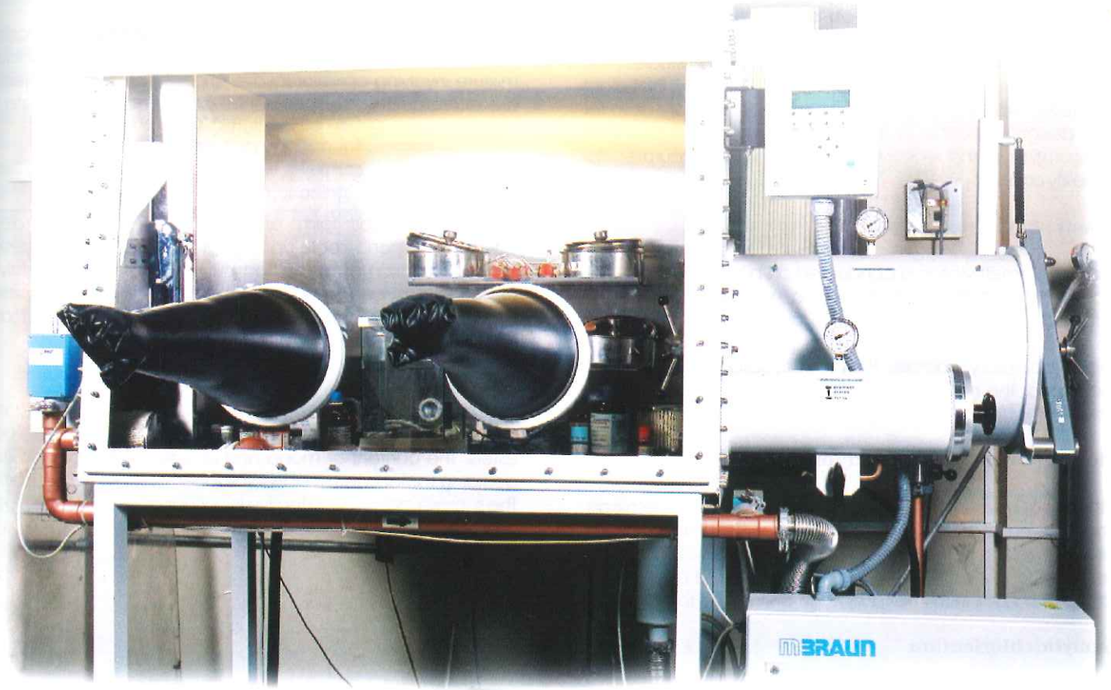




6.7.6 Crystallization of poly(1-butene)

poly(1butene) (PB) is known to exhibit time dependent polymorphism. The phase transformation of the meta-stable tetragonal form II to stable hexagonal twined crystal form I starts after the crystallization of the form II the kinetics of which are influenced by pressure, temperature, and mechanical deformation. The formation of intercalated PB/ clay nanocomposites affects this phase transformation. The process was accelerated in the intercalated nanocomposites as compared to pristine PB. The figure shows the accelerated process.





7. Process development and engineering

The Process Development and Engineering group plays the pivotal role in translating laboratory processes to commercial technologies by combining novel process chemistry with advanced pilot plant studies and process engineering. The group also assists the chemical process industry to achieve efficient in terms of efficient, eco-friendly and trouble-free operation by providing R & D inputs. In order to meet these objectives the group undertakes process design & development, rigorous pilot plant studies, providing assistance in plant commissioning, troubleshooting and conducting feasibility study at various stages of R& D to substantially reduce the time taken for moving processes from flask level to commercial scale, the group provides concurrent engineering inputs to bench scale process development work.

7.1 Catalytic processes

Acylation

Catalytic acylation reactions were conducted on pilot plant scale. The experiments were conducted using a novel reactor configuration. Optimal operating conditions were determined based on several parameter variations in smaller laboratory reactors. The experiments were demonstrated to the industrial customer. The product obtained was isolated and tested. The novel process of catalytic Friedel-Crafts reaction is a good replacement for the classical process, which is currently widely in practice.

Pilot plant reactors: Time-on-stream studies

In the use of zeolite catalysts in the preparation of fine chemicals, time-on-stream data and deactivation studies play an important role in development of the technology. Pilot plant has proved with a fair degree of accuracy necessary data for plant design. Life cycle of the catalyst is enhanced by better configuration of the reactors and is estimated accurately for feasibility analysis.

Vapour phase O-methylation

Catalytic O-methylation is conducted on pilot plant scale. The experiments are conducted using a number of recipes of catalysts and reactor configuration and optimal parameters are determined based on several parameter variations in smaller laboratory reactors. The product obtained was isolated and tested. The novel process of catalytic reaction is a good replacement for the classical process, which is in practice.

Pilot plant reactor: Life study of catalysts

In the use of novel catalysts in the preparation of fine chemicals, time-on-stream data and deactivation studies play an important role in development of the technology. Pilot plant is expected to generate data for plant design. Life cycle of the catalyst is enhanced by better configuration of the reactors.

Catalytic chlorination

Selective, catalytic chlorination of toluene using a proprietary catalyst is demonstrated to a customer at his site.

7.2 Process design & engineering

The division is equipped with the latest software for process simulation and engineering drafting. The simulation software is used to do mass and energy balance calculations, process design of heat exchangers, pumps etc. and to determine physical properties of process streams involving solids, liquids or vapours.

Process know-how documents and Basic Engineering Packages (BEP) can be prepared incorporating process flow diagrams (PFDs) and piping and instrumentation diagrams (P & IDs) with the available software

Basic engineering package (BEP) for a novel multiphase reactor

Preparation of BEP for a pilot plant using liquid phase hydrogenation technology and a novel continuously operating hydrogenation reactor is completed. This program is undertaken with an industrial partner as a sponsoring party. Catalyst development, process development and product validation were undertaken as bench scale work. A high-pressure reactor with four phases is a crucial equipment in the whole scheme. The sponsoring party has shown interest in putting up a pilot plant for the novel hydrogenator. Customer is assisted in finer design and installation of the pilot plant facility.

Simulation studies: Separation operations

A process simulation package is used to generate a feasible process flow sheet for separation of a complex, non-ideal liquid mixture involving epichlorohydrin and allyl chloride. The results are combined with experimental phase equilibrium data to design an appropriate separation scheme.

7.3 Pilot plants

Pilot plant studies form an essential step in technology development and scale-up. The group specializes in design and construction of dedicated pilot plants involving catalytic oxidation, amination, acylation and hydrogenation processes. Such an assignment includes preparing P & ID, sizing and equipment selection.

Sucrose ester

Sucrose esters are non-ionic surface-active agents manufactured from pure sugar and vegetable oils / fatty acid esters. The content of mono and di-esters in the product is a deciding factor in terms of its hydrophilic or lipophilic properties. The sucrose esters are effective in various applications like food, cosmetics and pharmaceuticals.

A solvent-less process for the preparation of sucrose esters was developed by a Pune based sugar institute on a laboratory scale of 0.5 to 1.0 gm mole of sucrose. The industrial customer subsequently entered into an agreement with NCL for a basic engineering package for pilot plant based on their process. Lab scale demonstration of the process was studied and modifications were suggested. This modified protocol was used for the preparation of the basic engineering package. Objective was to provide a basic design document to the customer for further scale-up and experimental studies at their site

The customer was assisted in commissioning the pilot plant. Presently, the trial of preparing sucrose ester is in progress and would be completed in a couple of month's time.

7.4 Plant commissioning, de-bottlenecking and troubleshooting

NCL has acquired vast experience in these aspects by constant interaction with plant engineers, equipment vendors / suppliers and project engineering groups. Section-wise / stage-wise testing of a process and commissioning of all equipment / machinery is done by observing all the protocols of plant start-up.

7.5 Feasibility study/ analysis

This is done at various stages of R& D, starting from scanty preliminary data and conceptual flow sheeting to post-pilot plant and advanced engineering stage. It was done for some polymer additives and specialty chemicals.

A specialty monomer plant

NCL provided assistance to commission 900 TPA specialty monomer plant (ATBS) and stabilize its operation by continuous monitoring of the plant performance. Bottlenecks were identified and remedial actions were recommended. This plant is currently operational at 125% of its rated capacity.

8. Public - private partnership programmes

NCL plays a lead role in several major collaborative projects with private industries under the auspices of New Millennium Indian Technology Leadership Initiative Programme (NMITLI) and Department of Science & Technology (DST). NMITLI programmes are chosen after extensive consultations amongst stakeholders and are undertaken in mission mode and a time bound manner.

8.1 NMITLI Projects

8.1.1 Sulphur removal from petroleum fuels using nanoparticulate catalysts *(Chennai Petroleum Corporation Ltd, Chennai and Sud Chemie India Ltd, New Delhi)*

The aim of this research project is to develop a catalyst and a process for the deep desulphurization of diesel to bring down its sulphur content to less than 50 ppm at the typical operating conditions used in Indian refineries. Both Co-Mo and Ni-Mo based catalysts were successfully prepared in the laboratory scale (100 g) which could desulfurize diesel to <50 ppm at a pressure of 40 bars. Catalyst scale-up is in progress and commercial trials in CPCL are contemplated.

8.1.2 Five & 25 kW decentralized power packs *(Bharat Heavy Electricals Ltd, Hyderabad, Sud Chemie India Ltd, New Delhi, and SPIC Science Foundation, Chennai)*

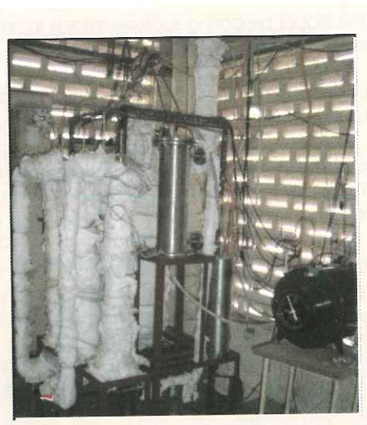
Fuel cells are the promising candidates for truly energy-efficient and more environment friendly power generation devices. Fuel cell comprises a family of multidisciplinary technologies. NCL has formed a virtual team of the scientists from disciplines like organic chemistry, membrane science and technology, catalysis, materials science and process development.

Fuel cells are commonly classified by the type of electrolyte used. Work is being carried out on Polymer Electrolyte Fuel Cell (PEFC) or Proton Exchange Membrane Fuel Cell (PEMFC). PEMFC has a solid-polymer electrolyte with excellent resistance to gas crossover. PEMFC can operate at high current densities, which offers low weight, cost and volume. The main disadvantages are poor resistance to CO tolerance and low operating temperature. The CO tolerance can be managed by reducing the CO content in H_2 by using the appropriate catalytic process. Alternatively, the membranes that can be operated at high temperature may be used so that the CO tolerance capacity can be improved. The major components of the fuel cell power pack are: **fuel processor**, **fuel cell stack**, and **power conditioner**.

Fuel processor is an integrated unit used for the conversion of LPG to a fuel gas reformate suitable for the fuel cell anode reaction. Fuel processing encompasses: (i) raw cleaning removal of sulphur, halides and ammonia, (ii) raw fuel conversion- converting a hydrocarbon fuel to a hydrogen rich gas reformate, and (iii) reformate gas alteration - converting carbon monoxide and water in the fuel gas reformate to hydrogen and carbon dioxide via the water gas shift reaction and selective oxidation to reduce CO to a few ppm. The hydrogen rich product and air (oxygen) are fed to fuel cell stack to generate electricity. The steam reformer (SR) and preferential oxidation (PROX) catalysts were developed. The know-how for scale-up (kg size) of SR catalysts has been transferred to the industrial collaborator. The catalyst is giving an excellent performance in terms of conversion as well as hydrogen yield. Preparation of platinum based PROX catalyst was scaled up to 500 g size at catalyst pilot plant.

Proton exchange membrane (PEM) is a key component of fuel cell stack. The monomer, diaminobenzidine (DAB), is prepared from readily available starting material at lab scale by new catalytic routes. Synthesis of a polymer, polybenzimidazole (PBI), from DAB and further synthesis of PBI based PEM is optimised and alternate novel routes are being explored.

A fuel processor with a capacity to produce 4000 LPH of hydrogen was designed. It was operated for 830 hours. The fuel processor was evaluated using Ni based steam reforming catalyst and Pt based PROX catalysts. Commercially available HTS and LTS catalysts were used. HTS, LTS, PROX reactors were designed and operated as adiabatic reactors. CO concentration in reformate gas after HTS was reduced to 2 per cent and after LTS it was 0.2-0.5 per cent. The reformate gas was sent to PROX reactor with 150-200 per cent excess air. The CO concentration after PROX was reduced to 0-20 ppm. In the fuel processor, 93 per cent conversion of LPG was obtained.



8.1.3 A catalytic process for the preparation of acetic acid and ethylene through vapour-phase oxidation of ethane *(Indian Petrochemicals Corporation Ltd, Vadodara)*

Alkanes, especially the light ones such as CH_4 and C_2H_6 are abundantly available in nature. At present, acetic acid is produced from these hydrocarbons via the syn-gas route ($CO+H_2$) or ethylene. A much simpler and more economical route will be the direct oxidation of ethane with O_2. Research is in progress towards accomplishing the direct conversion of ethane to acetic acid.

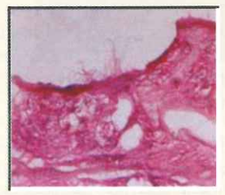
8.1.4 Detergent alcohols by oxidation of higher alkanes using alkyl hydroperoxide as oxygen carrier *(Indian Petrochemicals Corporation Ltd, Vadodara)*

The use of biodegradable alcohol based detergents is gaining importance the world over, in a major move from the conventional detergents like LAB sulfonates. In India the utilization of the biodegradable detergents is still in its infancy and is expected to increase in future. So far the manufacture of detergent alcohols in India is via hydrogenation of fatty acid esters. An alternate cheaper route could be via oxidation of the abundantly available C_{11}- C_{13} alkanes. In this program it is proposed to develop a process for the manufacture of detergent alcohols by the oxidation of corresponding alkanes mixture (C_{11}-C_{13}) using t-amyl hydroperoxide (TAHP) as an oxidant. The unutilized C_5 fraction from refineries (containing a mixture of pentane and isopentane) will be employed to generate the TAHP, which after transfer of the oxygen yields t-amyl alcohol (TAA), an important commercial product. The cleavage of the alkyl hydroperoxides to obtain desired oxygenated products would also be assessed.

The investigations on oxidation of decane and dodecane have resulted in the development of new catalysts for the reaction using TBHP as the oxygen carrier. Studies have also indicated the possibility of oxidation of higher alkanes using molecular oxygen, which also yields the desired alcohols and ketones. Currently work is in progress on the oxidation of alkane mixture available commercially and also on the preparation of TAHP via isopentane oxidation.

8.1.5 Biotechnology of leather: Towards cleaner processing *(SPIC Science Foundation, Chennai)*

Leather industry generates enormous amounts of solid as well as liquid wastes causing ground and water pollution. Many tanneries were forced to close down on account of pollution and are now switching over to cleaner methods of leather manufacture. Dehairing of skins and hides is one of the major sources of pollution. Enzymatic method of dehairing as an alternative to chemical method is gaining world-wide attention. A fungal strain isolated at NCL secreting high levels of alkaline protease in short fermentation cycles was evaluated at CLRI, Chennai for its application in leather manufacture. The dehairing of goat/ sheep skins and cow/ buffalo hides in absence of sulfide using NCL enzymes have been demonstrated in commercial tanneries.



Dehairing with lime sulphide

Dehairing with NCL alkaline protease

Based on the positive results obtained, newer sources of proteases and lipases with properties suitable for application in leather manufacture have been screened. Two proteases have been selected as lead enzymes for further scaling up and large scale evaluation trials.

8.1.6 Microbiological conversion of Erythromycin to clarithromycin and other novel biologically active molecules *(Alembic Chemicals, Vadodara, Institute of Microbial Technology, Chandigarh and Regional Research Laboratory, Jammu)*

Clarithromycin (6-O-methoxy erythromycin) is a semi-synthetic analogue of erythromycin having enhanced activity profile compared to the parent compound. At present, it is synthesized chemically from erythromycin involving multistep reaction sequence that requires protection and de-protection steps, thus reducing the overall yield to 30 per cent. The steps of protection and de-protection make the process lengthy as well as costly.

The fact that microbiological processes are simple, environment friendly as well as functional or site specific make them more attractive for carrying out otherwise difficult transformations. Several microbial processes compete successfully with chemical processes in the transformation of steroids, β-lactam, amino acids and peptides. Since the conversion of erythromycin to clarithromycin involves only O-methylation at C-6 hydroxyl group, there is a likelihood of effecting this transformation microbiologically in single step.

The project deals with the extensive screening of microbial strains for above-mentioned conversion capable of performing O-methylation at desired C-6 position. The project also deals with the possibility of formation of novel analogues of erythromycin possessing improved or different antibiotic activity profile than the parent molecules, erythromycin. During the project 1123 bacterial strains and 144 fungal strains were screened. No strain was found capable of transforming erythromycin to clarithromycin. However, three strains were found to produce acid stable metabolites, which were antibacterial in nature as confirmed by bioassays.

8.1.7 Stimuli sensitive polymeric nanoparticle based advanced drug delivery systems for cancer, diabetes and antibacterials *(Sri Chitra Tirunal Institute of Medical Sciences & Technology, Trivandrum and USV Ltd, Mumbai)*

Many biologically active peptides and proteins are now available for clinical use and are being investigated as biopharmaceuticals. It is well known that parenteral route is the only viable route for administration of such drugs. But the patient and physician always prefer oral delivery of the drugs because of ease of administration. Oral administration is the most attractive route for most of the drugs. The major problem associated with the oral delivery of these biologically active

compounds is degradation of biologically active compounds in the presence of the enzymes secreted in the gastrointestinal (GI) region and also poor absorption due to polar nature and size. For the development of oral delivery systems, the biological and physical barriers of the GI tract must be traversed before a polypeptide can reach its specific target within the body. So there is a need to stabilize protein and peptide against all physiological barriers.

The objective of the work was to stabilize biologically active protein and peptide, against proteolytic enzymes, gastric and intestinal secretions, temperature as well as common organic solvents used in micro-encapsulation. Another objective is to synthesis a new class of biodegradable, stimuli sensitive polymers as a carrier for oral delivery of proteins and peptides.

The proteins and peptides against proteolytic enzymes, gastric and intestinal secretions, and temperature as well as common organic solvents used in micro-encapsulation were stabilized. New class of stimuli sensitive polymers was synthesized. Drug was encapsulated into polymeric nanoparticles. Morphology and release profile of nanoparticles was studied and some of these polymers were used as a carrier for delivery system of suitable drug. A method for stabilization of Insulin was developed, which can be applied for other proteins and peptides. Polymers synthesized are useful for oral delivery system of Insulin. These polymers can be used for gastro retentive and test masking of bitter drugs.

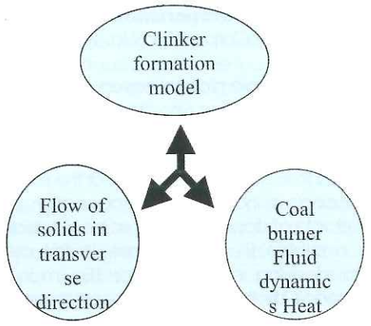
8.1.8 Improved granular processing: towards energy efficiency and resource conservation in cement manufacture *(Grasim Industries Ltd., Mumbai, Indian Institute of Technology, Mumbai, Larson & Toubro Ltd., Mumbai, National Metallurgical Laboratory, Jamshedpur, The Associated Cement Companies Ltd., Thane and The India Cements Ltd., Chennai)*

A multi-layer modelling framework is being developed to generate computational tools to understand and to enhance performance of cement rotary kilns.

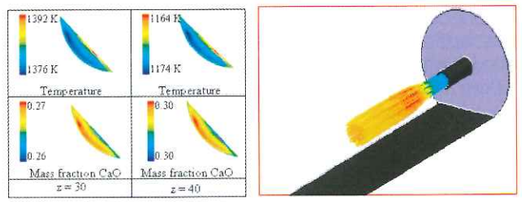
CFD Model for rotary cement kilns

The performance of a cement plant largely depends upon performance of rotary cement kilns, making it the key component in a cement industry. A programme is initiated to develop a comprehensive computational model capturing following features simultaneously for a rotary cement kiln.

- Complex fluid flow as the solids travel along the length of the kiln.
- Clinker formation along kiln length formed by a series of complex solid decomposition, solid-solid and solid liquid reactions along the kiln length.
- Heat transfer that occurs between freeboard, bed and kilns walls by all the three modes of heat transfer i.e. Conduction, convection and radiation along with kiln shell losses.



Parametric grid was generated for the entire kiln, which was split into two parts: a freeboard region and a bed region. Based on these, flow, heat transfer and chemical reactions occurring in the freeboard and the bed regions were modelled separately. Discrete solid particles in the bed region were treated as incompressible pseudo-homogeneous fluid. For simulating flow in the bed region, a constant viscosity was specified. The models for predicting motion of solids using granular theory approach are in initial stages of development and will be incorporated in model in the near future. A computational model based on a Eulerian-Lagrangian approach was developed to simulate freeboard region. The motion and burning of coal particles was modelled using a Lagrangian approach. The gas phase combustion was modelled using finite rate chemistry and radiation was modelled using the P-1 approach.



Typical results obtained from the bed and freeboard run

The bed model was first solved with some initial heat flux boundary condition specified at the interface between the bed and the free board region. The free board was then simulated using temperature profile obtained from the converged bed run to get the heat flux profile at the interface. This process was continued till the temperature and the heat flux at the interface no longer changed with further iterations. Suitable under relaxation factors were identified to accelerate the convergence of the coupled simulations.

The model satisfactorily predicts the behavior of rotary cement kilns and is the most realistic model for rotary cement kiln as it considers flow, reactions and heat transfer simultaneously. Detailed sensitivity study is now in process to develop energy efficient operating protocols for kiln operation thereby enhancing the performance of rotary cement kilns.

In addition, i) A one-dimensional model for rotary cement kiln based on phenomenology to understand the overall kiln behavior and calibrate the CFD model, ii) CFD Models for transverse plane in rotating kilns and iii) a CFD model to study heat transfer in transverse plane of rotary kiln were also developed.

8.1.9 Biodegradable plastics from agricultural wastes: cellulose esters based on bagasse derived cellulose *(Central Pulp and Paper Reserach Institute, Saharanpur, EID-Parry Ltd., Chennai, Godawari Sugar Mills/Somaiya Organic Chemicals Group, Mumbai, Reliance Industries, Mumbai and Thapar Centre for Industrial Research and Development, Patiala)*

Agriculture by-products constitute one of the most important class of renewable and sustainable feedstocks for the production of polymeric materials. Considerable research efforts, encompassing diverse disciplines, such as microbiology, genetic engineering, enzyme catalysis, and polymer science, have been invested into developing viable technological solutions for new materials based on renewable resources. In spite of world-wide attention being paid to the area of sustainability in the production and consumption of materials, polymeric materials derived from agricultural products are not yet commercially competitive with petrochemical based polymers. There are several reasons for this, the most significant being, relatively poor energy efficiency of bioconversion processes, distributed availability of agricultural by-products and their cost of transportation, technology limitations in bioconversions and ability to tailor a wide range of material properties from a single polymer derived from renewable source. This has inhibited growth of large volume polymer industry based on renewable resources.

Steam Explosion Digester

Consequently, any material industry in India based on agricultural products must involve the use of appropriate feedstocks. Secondly, the products of such an industry must be of high value with potential global markets, so that there is sufficient commercial incentive for its manufacture. The emphasis has been on fractionation of agricultural biomass like sugarcane bagasse to yield all three major component polymers cellulose, hemicellulose, and lignin. A steam explosion process has been successfully demonstrated for accomplishing this separation. Further, value-added derivatives like cellulose in acetate and lignosulfonate was prepared from bagasse derived cellulose and lignin, respectively.

8.1.10 Value added polymeric materials from renewable resources: lactic acid and lactic acid based polymers *(Central Food Technological Research Institute, Mysore, Central Salt & Marine Chemical Research Institute, Bhavnagar, Godavari Sugars Pvt. Ltd. (Somaiya Group of Industries), Mumbai, Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Technology, Bombay, Prathishta Biotech Industries Pvt. Ltd, Hyderabad and Reliance Industries Ltd, Mumbai)*

Lactic acid and its derivatives are widely used in food, pharmaceutical, leather and textile industries. Recently, there is an interest in lactic acid to be used as a raw material for the production of polylactic acid, a polymer used as specialty medical and environment-friendly biodegradable plastic. Lactic acid is produced commercially either by chemical synthesis or by microbial fermentation. Chemical synthesis from petroleum feedstock leads to production of racemic DL-lactic acid, whereas fermentative route from renewable carbohydrates results in the production of desired stereo-isomer, optically pure L(+)- or D(-) lactic acid. The production of optically pure lactic acid is essential for polymer synthesis in which lactic acid is used. In addition, optically pure L(+) lactic acid is polymerized to a highly crystalline polymer suitable for fibre and oriented film production.

The main objective of the project is to identify suitable strains of *Lactobacillus* and to improve its performance in relation to lactic acid production. We have identified a *Lactobacillus* strain capable of producing L(+) lactic acid with good productivity (1.4g/l/h). We have improved this strain using traditional approaches and were able to get a mutant strain capable of producing L(+) lactic acid with better productivity (3.0g/l/h) at pH 6.5. The strain is able to grow in a medium with minimum amount of yeast extract, which reduces the cost of lactic acid production. Optimizations of nutritional requirements and fermentation parameters (at a 10 litre scale) have been achieved.

8.1.11 Defunctionalization of carbohydrates as a feedstock to manufacture industrial chemicals *(Agharkar Research Institute, Pune, Anil Starch Products, Ahmedabad, Gujarat Narmada Fertilizer Corporation, Bharuch, Indian Institute of Technology, Madras, Indian Institutes of Chemical Technology, Hyderabad, Mumbai University Department of Chemical Technology, Mumbai, Prathista Industries Ltd., Secunderabad, Regional Research Laboratory, Jammu, Regional Research Laboratory, Trivendrum, Tamil Nadu Petro Products Ltd., Chennai, Tata Energy Research Institute, New Delhi and University of Delhi, South campus, New Delhi)*

(S)-3-Hydroxy-γ-butyrolactone (HGB) is an important synthetic intermediate for a variety of chiral compounds and in the synthesis of range of pharmaceuticals including a product for reducing the cholesterol i.e. Atorvastatin, a cancer treatment, a dietary supplement, an analgesic, an AIDS treatment and an antibiotic. Defunctionalisation of carbohydrates has been attracting much attention as a vibrant synthetic tool for the enantioselective synthesis of variety of compounds. HGB has been synthesized by using inexpensive readily available carbohydrate materials such as maltose, maltodextrin. A carbohydrate source was treated with cumene hydroperoxide in the presence of base which led to the formation of (S)-3,4-dihydroxybutyric acid and glycolic acid. The subsequent acidification with an acid and removal of solvent afforded the desired butyrolactone in about 50 per cent yield. The new process developed offered a practical and cost effective route and would have advantages since it avoids use of expensive starting materials.

8. 2 Drug development projects

The following projects were undertaken at NCL under the collaborative R&D programme for drug development funded by DST.

8.2.1 Synthesis of selective cyclo-oxygenase 2-inhibitors and a novel symbiotic approach to anti-inflammatory and immunomodulatory therapy

(Glenmark Pharmaceuticals Ltd, Mumbai)

The main objective of this project is to evolve symbiotic therapy for chronic inflammatory disease like rheumatoid arthritis through a novel approach towards initial systemic relief by inhibition of specific inducible cyclooxygenase-II enzyme and arrest degeneration of cartilage and bones by normalizing array immune system through immunomodulation.

The project was initiated with the objective to synthesize highly selective COX-2 inhibitors by the molecular variation of presently known and effective COX-2 inhibitors, and design the synthesis of compounds having anti-inflammatory and immuno-modulatory activity in a single molecule. The therapeutic potential of these molecules will be tested for other immune disorders.

This year one hundred eight new chemical entities (NCEs) were synthesized and sent to Glenmark for screening the biological activity. From screening studies of new Nimesulide analogues it was observed that few compounds [GRC-7078 (NCL-VV-03), GRC-7133 (NCL-SG-3A), GRC-7132 (NCL-PP-374) GRC-7068 (NCL-PP-229)] showed promising anti-inflammatory activity. These NCEs belong to new category of compounds which is to be explored for possible lead compounds for new anti-inflammatory agents.

8.2.2 New anticancer compounds: Design, synthesis, screening and optimization through QSAR

(Dabur Research Foundation, Ghaziabad, Indian Institute of Chemical Biology Kolkata, Indian Institute of Chemical Technology, Hyderabad and University of Hyderabad)

Synthesis of combretastatin A-4 (CA-4) analogues was undertaken. Novel molecules were designed considering the SAR reported for CA-4 which required *cis* restricted geometry of the double bond joining the two aryl groups. Initial studies on the molecules of cyclopentenones, furanones and tetralones encouraged us to continue our efforts in the same direction so as to select some hit molecules and finally the lead molecule as potential anti-cancer compound. The compounds from all three categories showed potential cytotoxic activity. Overall fifteen molecules were selected as hit molecules and four of them have been submitted for pre-clinical studies.

8.2.3 Design, synthesis and biological evaluation of new antitubercular compounds

(Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Science, Bangalore, and Lupin Laboratories Ltd, Mumbai)

In search of new anti-tubercular drugs, NCL and IICT, Hyderabad worked together towards design and synthesis of new compounds in a semi-combinatorial mode. During this year, about thirty five new compounds were synthesised and submitted to the industrial collaborator for screening against various strains of mycobacterium *in vitro and in vivo*.

8.2.4 Synthesis of selective β_3 adrenergic receptor agonists as a novel therapy for obesity

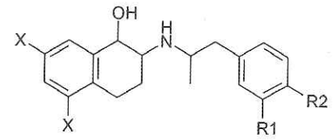
(Central Drug Research Institute, Lucknow, Glenmark Pharmaceuticals & Research Centre, Mumbai and Indian Institute of Chemical Biology, Kolkata)

The project is aimed at the synthesis of a number of new chemical entities and to identify compounds that show considerable anti obesity properties. Obesity is metabolic disorder caused by chronic imbalance in the energy balance equation. Medical treatment of obesity becomes a necessity when prevention fails.

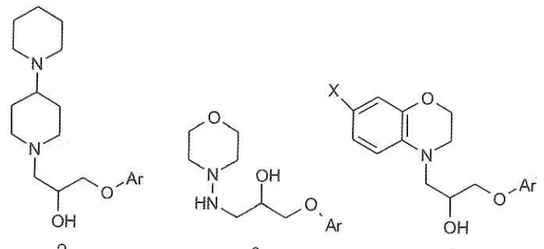
The principal objective of this project was to achieve significant advancement in obesity therapeutics by synthesizing novel chemical entities having specific β_3-adrenegic receptor agonistic properties. Targeting β_3-adrenegic receptor which is important site for energy storage and energy expenditure, for the reversal of obesity is a novel approach for the treatment of obesity. Discovery of specific β_3 -adrenegic receptor agonists can serve as an excellent therapeutic target for obesity and obesity related disorders.

A number of NCEs belonging to the following structures (**1**, X= H or Br; R1 = H or OMe; R2= OH, OMe, NO_2, NH_2, OCH_2COOH etc)

were synthesised. Fourteen compounds of this skeleton having varying substitutions were prepared and submitted to the industrial collaborator. Seven of these compounds were found to be active.



In addition to the above a number of compounds belonging to the class of aryloxypropanolamines having structures shown below (**2-4**) were also synthesized (Ar denotes differently substituted phenyl or naphthyl groups and X denotes H or Br).



With the above synthesis, NCL has completed the synthesis of approximately eighty NCEs, thirty-nine of these were screened and seven were found active. The synthesis of the remaining compounds is in progress.

8.2.5 Design, synthesis and testing of new chemical entities as potential antifungal agents

(FDC Ltd, Mumbai)

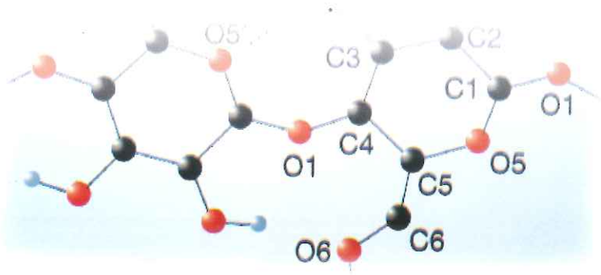
This project involves development of novel antifungal agents. The selected compounds are being synthesized in our group and sent to the industrial collaborator for screening of their potential antifungal activity. Three classes of compounds were selected to develop new chemical entities related to fluconazole, voriconazole and sapidolide. Accordingly, this year, thirty-five compounds have been synthesized at NCL and screened for antifungal activity by the industrial collaborator. Most of the compounds have shown antifungal activity. Five compounds selected on the basis of antifungal activity exhibited by them, have been synthesized on five gm scale and sent to the industrial collaborator for toxicity studies. One of the novel compounds has been shown to be nontoxic and is undergoing further biological activity studies. Synthesis of more NCEs is in progress.

8.2.6 Latent *M.tuberculosis*: New targets, drug delivery systems and bioenhancers and therapeutics

(Bose Institute, Kolkata, Central Drug research Institute, Lucknow, Centre for DNA Fingerprinting and Diagnostics, Hyderabad, Indian Institute of Chemical Technology, Hyderabad, Indian Institute of Science, Bangalore, Institute of Genomics and Integrative Biology, Delhi, Lupin Laboratories Ltd, Mumbai, Regional Research Laboratory, Jammu, Tuberculosis Research Centre, Chennai and University of Hyderabad)

Tuberculosis, caused by *Mycobacterium tuberculosis*, is the greatest single infectious disease and is attributed with killing two million people annually worldwide. Estimates indicate that one-third of the world population is infected with latent *M.tuberculosis*. The synergy between tuberculosis and the AIDS epidemic, and the surge of multi-drug resistant clinical isolates of *M.tuberculosis* have reaffirmed tuberculosis as a primary public health threat. These bacteria are resistant to the entire antibiotic armoury including vancomycin-the so-called antibiotic of last resort. The recent emergence of drug resistant strains of TB is also of special concern. Over the past decade, significant advances have been made in the discovery and development of antimicrobial agents in general. However, the need for safe, microbially selective and effective antitubercular drug is apparent, and certainly no ideal agents with new mechanism of action have yet been developed.

NCL has initiated work on the new drug discovery (NDD) in the area of anti-tubercular drugs. Our goal is to synthesize New Chemical Entities (NCEs) and submit them to the industrial collaborator for evaluating anti-tubercular activity. Seventy-nine NCEs belonging to oxazolidinone class of compounds incorporating various nitrogen, sulfur and oxygen heterocycles were synthesised.



Catalyst pilot plant

Catalyst pilot plant facility has the capacity to produce a range of solid heterogeneous catalytic material such as zeolites, silica-aluminas, binary oxides and supported metal catalysts used in a range of industrial processes for petroleum, petrochemical, organic/ fine chemicals and detergent industries. The facilities for synthesis range from gram scale to a few hundreds of kilograms.

Mission and goals

- Development and optimization of cost-effective synthesis of zeolites and other solid catalysts
- Scale up, preparation and supply of catalysts based on NCL know-how
- Custom-made synthesis of zeolites and other solid catalysts

Competencies

Synthesis of zeolites and oxides

- Zeolites (ZSM-5 series), TS-1/ TS-2 (Titanosilicates), Beta (Al, Ti, Sn), LTL, FAU, P)
- SAPOs, Oxide / mixed oxide catalysts
- Fly ash based zeolite catalysts (A, ZSM-5, Beta etc.)
- Catalysts preparation and scale-up (up to 100 kg Powder Per batch at our Catalyst Pilot Plant, a unique Facility)
- Zeolites, Mesoporous (MCM-41, MCM-48, SBA, Carbon) materials, organo-inorganic mesoporous Materials and metaloxides

Processing and shaping of solid Catalysts

- Mixing and ball milling of catalyst powder
- Extrusion of the catalyst with chosen binder. Solids powder can be shaped in the form Of tablets, hollow spheres, balls, etc.

Infrastructure

- Reaction vessels with 20 L, 50 L and 1000 L capacity
- Spray dryers (3 kg/h and 30 kg/h), Pug Mill / Mix muller (25 kg/batch), Sigma Mixer 15-20 kg/batch, Mixtruder (25 kg/h) Calciner (700 °C, 60 - 100kg/batch &1000 °C, 20 - 25 kg/batch), Neoprene-lined ball mill (25-30 kg)
- Granulators with variable speed, Laboratory Extruder / Hand operated extruder, Solid cylindrical Tablet making machine, Ring cylindrical tablet making machine

Glimpses of current research

Scale-up of titanium silicate (TS-1) catalyst

The scale-up of TS-1 and its regular production at Catalysis Pilot Plant up to ca. 100 kg per batch (in 1000 L Reactor) is achieved and is being supplied to a Multi National Companies for Pilot Plant trial. TS-1 is a high-tech catalyst and presently is not available on commercial basis. This high value catalyst is a unique catalyst for (i) phenol to catechol and hydroquinone, (ii) propylene oxide by epoxidation of propylene, (iii) epichlorohydrin by the epoxidation of allylchloride, and (iv) production of heterocycles like pyridines and substituted pyridines.

Converting flyash into eco-friendly catalysts

In recent years increasing concern has been expressed about the potential of human activities to alter the Earth's climate and its atmosphere. The future poses challenges to the scientists, technologists and engineers towards sound management of fly ash disposal and deposition technologies. Fly ash, which is a byproduct of coal burning, contains mostly aluminosilicates. The fly ash, an otherwise waste material was converted into a useful cost-effective and eco-friendly zeolite catalyst. The fly ash was collected from a Thermal Power Station, situated at Parali (Maharashtra). It has been demonstrated that zeolite beta can be prepared using fly ash.

Reactors used for the synthesis of flyash Based zeolite Beta

Center for materials characterization

The technological progress has been strongly influenced by the creation of new materials and further improvement of the existing materials. It is very important to understand the structure, microstructure, morphology' elemental composition (bulk or surface) while developing and using the new materials. Center for Materials Characterization is a well-equipped, central resource facility of the laboratory. The facilities at the Center include several major instruments, which are looked after by experts in the area providing a strong support to the Institute's major R & D programs. Apart from this, the Center also extends its technical services to outside research institutions, Universities and industries, builds its own research programs and trains young scientists and students.

Mission and goals

- To maintain and continually upgrade the infrastructural facilities at this largest resource center of NCL for providing high quality results
- To offer technical expertise in structural characterization and compositional analysis of materials that is important to the major R & D projects of NCL
- To extend the expertise and consultancy services to outside educational institutes and Industries
- To take up the research projects and contract research projects in the niche areas that are of commercial and basic research interest
- To train students and young scientists on the sophisticated instruments

Competencies

- Single crystal X-ray crystallography of small organic molecules and biomacromolecules
- Electron microscopy (scanning and transmission) of soft and hard materials
- Surface spectroscopy of catalytic, inorganic and polymer materials
- Mass spectrometry of organic and biomolecules
- X-ray diffraction of crystalline and semicrystalline Materials
- Measurement of magnetic properties of materials

Infrastructure

- Scanning Electron Microscope (SEM) - Leica 440 with EDAX- Phoenix model
- Transmission Electron Microscope (TEM) - JEOL 1200 EX
- Single Crystal X-ray Diffractometer - Smart Apex.
- Electron Spectroscopy for Chemical Analysis-ESCA 3000
- LC-MS, PE SCIEX, Qstar Pulser
- X-ray Diffractometer (Powder) - Philips PW-1830
- DTA/TG Thermal Analyser Model 32 SII and DSC 220C SII
- Laser Raman Spectrometer SPEX 1403
- Electron Spin Resonance (ESR) Spectrometer - Brucker
- Vibrating Sample Magnetometer - PAR Model No. 4500

Glimpses of current research

1. SEM with energy dispersive X-ray spectrometer

Scanning Electron Microscope (SEM) provides important information about topography, morphology, grain boundry, grain size, shape, distribution, voids, pores, flaws, cracks and homogeneity of the materials. SEM is having a high magnification and resolving power, therefore heterogeneous organic and inorganic bulk specimens can be examined on a micrometer and nanometer scale. It gives a three-dimensional appearance of the specimen image because of the large depth of the field. The Energy Dispersive X-ray Spectrometer (EDXS) with SEM provides specimen images with elemental analysis of selected features. It is very useful in observing in-homogeneities and imperfections in metals, crystals, ceramics, polymers, catalysts, rocks, minerals and colloidal nano-particles.

Star shaped $CaCO_3$ crystals appeared on cover page of Langmuir, **19** (2003), 10095-10099.

SEM: Leica Stereoscan 440 Computer controlled digital model

- Continuously variable high voltage (300V - 40 KV).
- Electron gun with tungsten filament.
- 5.0 nm resolution and 30x-300,000 x magnification in continuous variable mode.
- Secondary and back-scattered electron detectors.
- Manual Super - Eucentric stage, capable of handling specimens up to 200 mm diameter with 0 - 360 deg. rotational and 0-90 deg. tilt mechanisms.

- On line e-image acquisition and storage in TIFF files.
- Clean vacuum conditions using turbo pumping system.

EDXS: Phoenix EDAX

- Supper Ultra thin sapphire window Si(Li) detector with 135 eV resolution at 5.9 KeV.
- Detection of all elements starting with Boron.
- Standard less quantification software with Z, A, F corrections.

2. Single crystal X-ray CCD diffractometer smart apex

The diffractometer manufactured by Bruker-axs, Germany has the latest generation CCD detector having no fiber optic taper, which is highly sensitive 4K detector (170 e per photon) for small molecular crystallographic studies. This allows faster data collection on much smaller crystals (10 micron), which are poorly diffracting. The SMART APEX also makes it possible to make the measurements on highly unstable and various types of twinned crystals with the special software provided to tackle these data sets.

Smart APEX system

Smart APEX system has following special components

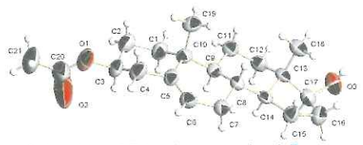
- D8 3-axis goniometer, K760 X-ray generator, Video Camera
- Frame buffer PC for data collection
- OXFORD Cryo System 700 series for low temperature data collection
- MZ-75 for crystal selection (with CCD and Photomicrography attachments to be added shortly)
- SHELXTL software for data collection, structure solution and refinement
- Graphics software for visualizing, plotting and analyzing the structure.
- The Cambridge Structural Database (CSD)

The single crystal X-ray crystallography facility is widely used by various research groups of NCL and there are interactions with outside CSIR laboratories, Industries and Universities. The knowledge of accurate molecular structures is a prerequisite for structure based functional studies. Crystallography can reliably provide the answers to many structure related questions, from stereochemistry, absolute configuration and molecular conformation to detailed bonding electron densities.

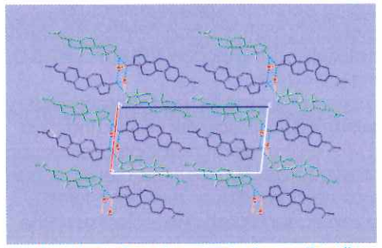
Natural products, drug molecules and polymorphism

Natural Products

Medicinally important natural products are of immense use. The single crystals of these compounds are normally very thin and it is difficult to assign molecular structures. With SMART APEX single crystal X-ray diffractometer, because of the highly sensitive detector, it has been possible to have diffraction data with a small crystal of size about 20 microns. 3β-Acetoxy-17β-hydroxy-androst-5-ene was isolated from aerial parts of *Acacia nilotica*. This Compound is the first example of steroid in the extract of *A. nilotica*. It showed anti-inflammatory activity.



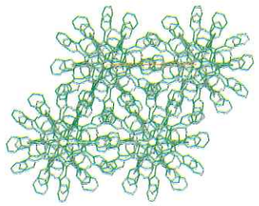
3-Acetoxy-17-hydroxy androst-5-ene



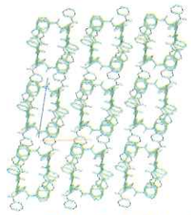
Packing of molecules in the unit cell

Polymorphism

The study of polymorphism exhibited by drugs is a frontier area of research having tremendous basic as well as commercial interest. The polymorphic and pseudopolymorphic behaviour of the cyclitol derivatives is being investigated. Two solvent free polymorphs of compound hexabenzoate are shown below:



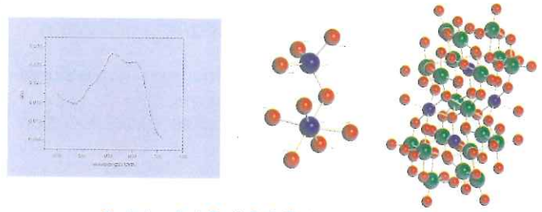
Needles in Hexagonal Space Group $P6_5$



Plates in Triclinic Space Group P-1

Catalysts and intermediates

The poly oxometalates act as dioxygenase catalysts. They have the ability to coordinate and activate dioxygen, catalyzing oxidation of a wide variety of substrates. A sandwich type polyoxotungstate, Na_{10} $[Co_4W_{19}O_{70}H_4]$ $44H_2O$, a mixed valence Co (II and III) oxometalate has been used for the catalytic oxidation of limonene with air and H_2O_2. ESR studies of the compound show antiferromagnetic properties. Co(III) atom in the tetrahedral coordination acts as the active site in the oxidation reaction.



Octahedral CoII-O & TetrahedralCoIII-O

Central NMR facility

Mission and goals

- Explore new avenues in methodology implementation for liquids and solids
- Apply NMR in a multi-nuclear multi-dimensional context
- Innovate and develop new structure characterization tools for materials applications
- Act as in-house resource center and interact with Industry
- Pursue activities towards advancement of fundamental knowledge in magnetic resonance

Competencies

- Solid and Solution State NMR methodology Development
- Structural Elucidation using modern NMR Spectroscopy
- Materials Science applications (polymers, molecular sieves, layered oxides, biomaterials)
- Inhouse instrumentation development
- Computational NMR (density matrix numerical simulations, powder spectral simulations and *ab initio* calculations)

Infrastructure

Centralized facility housing three supercon NMR spectrometers:

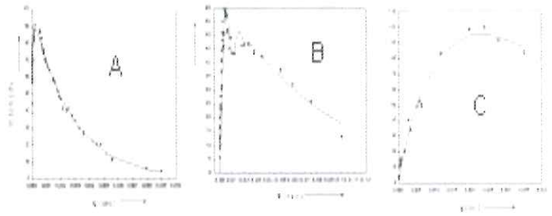
- 11.7 Tesla Bruker DRX-500 (with solids accessory)
- 7.0 Tesla Bruker MSL-300 (wide-bore solids with micro imaging accessory)
- 4.7 Tesla Bruker AC-200 (liquid state with auto sampler)
- DOTY Triple-Resonance high speed CP-MAS probe
- AMT 1 KW amplifier
- Probe-tuning and testing set up
- Silicon Graphics Work Stations (INDIGO2, `INDY, O2), Pentium IV Pcs

Glimpses of current research

1. Solid state NMR of polymers

Miscibility of blends

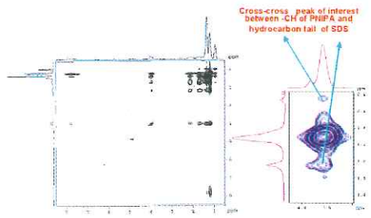
The dynamics of Cross-Polarization parameters (CP-Dynamics) and 2D wide line separation techniques have been employed to study the miscibility in blends of polystyrene and natural rubber. The CP behavior is distinctly different in the rigid (PS) and mobile (NR) phases, which is suitably manipulated through longitudinal mixing to enable spin-diffusion in the blend due to molecular mixing of the PS and NR domains. The molecular level miscibility is also reflected in the wide-line separation experiment. This has been exploited and further quantified to determine the domain size



^{13}C-^{1}H CP Dynamics of Polystyrene(A), Natural rubber (B) and the PS-NR Blend (C) (with longitudinal mixing of 50 msec). The signal evolution in C is for the same carbon (32 ppm) as in B.

Polymer-surfactant interactions

The association of SDS which suppresses the thermoreversible property (LCST) of polymer, poly *N*-isopropylacrylamide was followed by 2D NOESY and ROESY experiments. Evidence for molecular level interaction with the pendent isopropyl group and the hydrophobic tail of SDS was obtained.



500 MHz 2D NOESY spectrum of Poly N- isopropylacrylamide SDS(above CMC) mixture with 750 Ms mixing time in water and (C) (with longitudinal mixing of 100 msec).

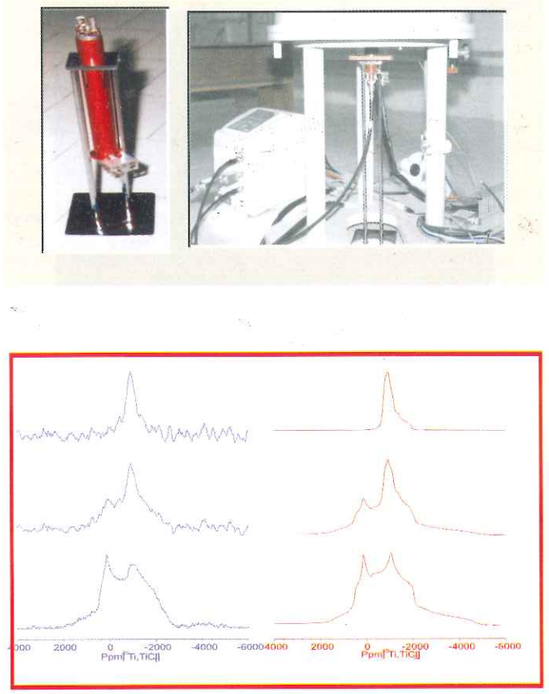
2. New structure characterization tools in catalysis science

Brönsted sites characterization through ^{27}Al 3Q-MAS and ^{1}H-^{27}Al REAPDOR

Rönsted and Lewis acid site characterization in molecular sieves is largely done using Temperature Programmed Desorption (TPD) and FT-IR techniques. However fine distinction among chemically similar, and yet structurally distinct, Brönsted acid sites, is hard to discern from these techniques. It was realized that the 'spin isolation' of protons in zeolites (NH_4^+, H^+ forms) would yield high resolution proton spectra at moderate spinning speed (10 kHz), allowing it to selectively recouple the heteronuclear dipolar interaction between the framework aluminum and the proton at the Brönsted acid sites. Experimental demonstration through Rotational Echo Adiabatic Passage Double Resonance (REAPDOR) NMR in partially ammoniated NH_4^+/H^+-Mordenite showed that structurally distinct Brönsted acid sites within $Q^4(3Si,1Al)$ environment can be clearly distinguished and the Al-H internuclear distance at the acidic sites experimentally determined.

$^{47,49}Ti$ NMR and heteroatom substitution in zeolites

In isomorphically substituted molecular sieves, using a variety of hetero-atoms, such as boron, gallium, vanadium, iron, titanium, etc, unequivocal evidence concerning the substitution of the hetero-atom in the framework structure is often sought using analytical techniques. With this in view, the hetero-atom substitution has been addressed through two different approaches: a) characterization of the hetero-atom environment based on changes in chemical shielding tensor and quadrupolar tensors for the nearest neighbor ^{29}Si and ^{27}Al sites; b) direct observation of the hetero-atom environment by NMR, using magnetically active nuclei, where present. The former approach has been demonstrated in the molecular sieve ETS-10 wherein the presence of a titanium next to a framework silicon renders the ^{29}Si chemical shielding tensor to become axially symmetric, thus providing the structural link for establishing hetero-atom substitution. In the second approach, direct observation of certain NMR active nuclei was limited to those possessing high natural abundance and/or larger magnetogyric ratios. The efforts were focused on a more challenging scenario, *viz.*, direct observation of NMR active nuclei with low natural abundance and low magnetogyric ratio. By using a very high magnetic field (11.74 Tesla) and spin-echo based NMR acquisition scheme, $^{47,49}Ti$ was brought into the realm of NMR observation and a study of titanium substituted USY (Ti-USY) was thus possible. This detailed work not only enabled to show that $^{47,49}Ti$ NMR is feasible as a characterization tool for the identification of the hetero-atom (titanium) environment in isomorphically substituted zeolites, but allowed to determine the chemical shielding and quadrupolar interaction parameters through a computer simulation procedure.

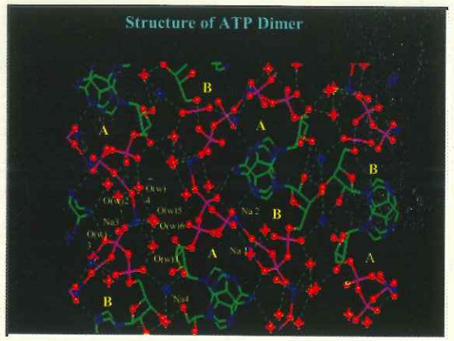


Home-built wide-line probe for $^{47,49}Ti$ NMR studies and the $^{47,49}Ti$ solid state NMR spectra recorded on static samples of TiO_2 (bottom) and Ti-USY (middle). The titanium environment in the zeolite USY is identified by spectral subtraction (top) and is fully characterized by computer simulations shown on the right.

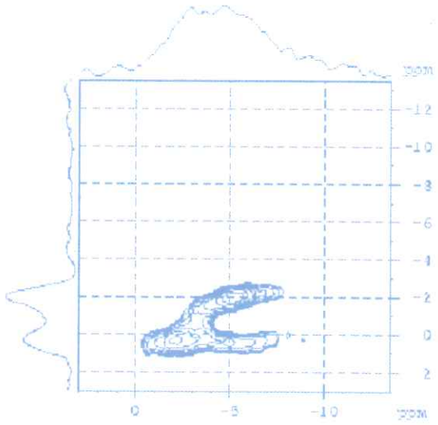
3. Solid state NMR of biomolecules

In an effort to apply modern solid state NMR techniques for the structural elucidation of biomolecules, ^{31}P MAS and ^{23}Na 3Q-MAS were employed to study the nucleotide, adenosine triphosphate (ATP) and adenosine monophosphate in their hydrated crystalline forms. For the ATP dimer, the six nonequivalent phosphorus environments in the crystal structure are fully revealed by ^{31}P MAS experiments, while the four sodium sites are fully identified from ^{23}Na triple quantum MAS experiments. *Ab initio* calculations of the ^{31}P chemical shielding tensors and the ^{23}Na electric field gradient tensors have been carried out in different basis sets using Gaussian 98W program.

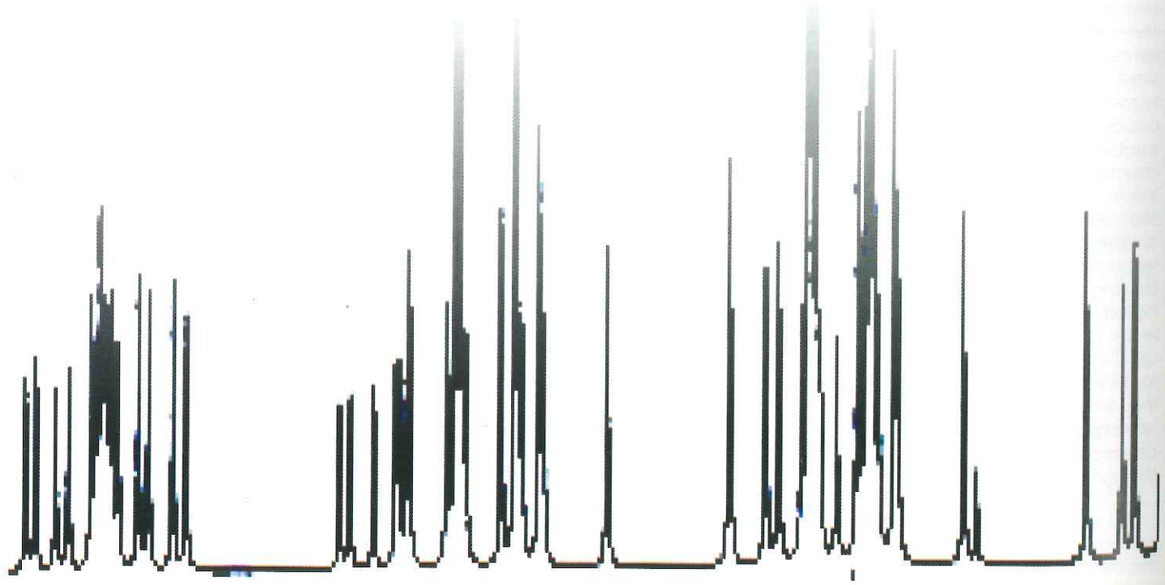
N an effort to apply modern solid state NMR techniques for the structural elucidation of biomolecules, ^{31}P MAS and ^{23}Na 3Q-MAS were employed to study the nucleotide, adenosine triphosphate (ATP) and adenosine monophosphate in their hydrated crystalline forms. For the ATP dimer, the six nonequivalent phosphorus environments in the crystal structure are fully revealed by ^{31}P MAS experiments, while the four sodium sites are fully identified from ^{23}Na triple quantum MAS experiments. *Ab initio* calculations of the ^{31}P chemical shielding tensors and the ^{23}Na electric field gradient tensors have been carried out in different basis sets using Gaussian 98W program.



Packing diagram of ATP dimer as viewed in the *ab*-plane showing the coordination of the four crystallographically nonequivalent sodium sites. These sites have been identified from ^{23}Na 3Q-MAS experiments.



^{23}Na 3Q-MAS contour plot of ATP.3H_2O, showing the resolution of sodium sites along the isotropic ω_1 dimension.



Combi chem-bio resource center

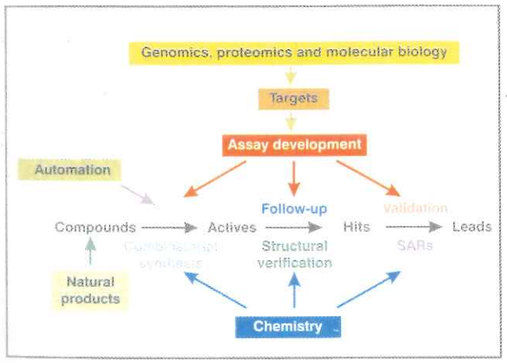
"Concept to Commercialization" in the drug discovery is a tedious and time consuming process, which generally takes more than 10 years. Minimum two million molecules have to be prepared and tested to get a lead molecule. In the last decade or so this process is accelerated due to several factors i.e., combinatorial techniques for the rapid generation of organic molecules, large availability of plants/ microbes with medicinal properties and high throughput screening. Combinatorial chemistry is a "State-of-the-art" technology which facilitates the rapid synthesis of organic molecules with a wide range of structural diversity. This, coupled with the natural product libraries and high throughput screening, will accelerate new drug discoveries and utilization of the vast natural biodiversity of India for value added products.

Mission & goals

- Compound libraries for lead discovery
- Medicinal plant processing based on activity
- Bio-assays for high throughput screening
- Newtargets for HTS assay developments
- Newmolecular scaffolds for specific diseases

Competencies

- Chemical synthesis of combinatorial libraries
- Bio-evaluation of medicinal plants
- Biological high throughput screening
- Chemoinformatics



Infrastructure

To cater these needs under one roof, a Combi Chem-Bio Resource Center has been established in NCL. All the equipments have been installed following globally accepted Good Laboratory Practice format. Besides Isothermal Titration Calorimeter (Micro-cal), the Centre has the following major equipments, ably supported by the essential analytical and other infrastructure facilities:

High throughput system (Beckman Coulter)

It is a totally robotic system including liquid handling system, radioactive and fluorescence detector, Co_2 incubator, shaker, etc. It can analyze ~5000 compounds per day.

organic parallel synthesizer (aswp 2000p, chemspeed)

Simultaneously 80 reactions, pressure 1-5 bar, temperature 70 to +150C, inert atmosphere, etc.

Accelerated solvent extractor (Dionex)

It can extract the plant material in 20 minutes, with solvent of our choice, with pressure, temperature and solvent programming.

Sepbox (Sepiatee)

Five gm of the mixture can be separated in 300-400 fractions in 24 hrs, thus avoiding the usual disadvantages associated with the chromatography of the natural products.

Simulating moving bed chromatography system (SMB, Knaur)

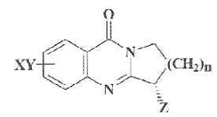
SMB enables substance mixture to be continuously separated and extracted in two fractions. Typically, the SMB process is set up in advance for a binary mixture and subsequently, each component can be immediately extracted in pure form. The advantages of SMB technology compared to classical batch chromatography include higher productivity, a 90% reduction in solvent consumption (on account of recycling), reduction in packing material cost by 80% and obtaining both the components of a binary mixture in higher concentration. The range of application includes: pharmaceutical chemistry (Chiral components e.g, steroids, peptides, antibiotics and other drugs), food chemistry (fatty acids, carbohydrated mixtures, i.e. sucrose/ molasses and fructose/ glucose), biochemistry (citric acid, phenylalanine), and petrochemistry (C8 hydrocarbon, i.e. xylene/ toluene).

Using SMB pilot unit CSEP C9116 and a method developed in house, both the enantiomers of a racemic drug were successfully separated. Feasibility study for three drug intermediates for a pharmaceutical company has also been done.

Glimpses of current research

Parallel synthesis

In search of new anti-fungal agents, NCL has developed a mini library of 100 acyl derivatives of variety of aromatic amines with various cyclic anhydrides using Chemspeed Parallel Synthesizer. An efficient four-step synthesis of naturally occurring anti-asthmatic agent (-)-vasicinone is being adapted to parallel synthesis of its analogues.



(n = 0 - 3)

X / Y / Z = H, alkyl, aryl, alkoxy, aryloxy, halo, nitro carboxy, hydroxy, amino, cyano, thio, sulfoxy, etc.

Using High-Throughput Extractor, Evaporator and Sep Box isolation of new natural products from rare indigenous plants identified under CSIR coordinated bioactive programme is in progress.

Natural product processing

Eighteen plants from the various biodiversity hot spots such as North Eastern India have been collected, identified and four of them have been processed using AS extractor and SEP box

High throughput screening

During this year, two assays have been optimized for automated screening. Glutamine synthetase is a target for screening anti tubercular agents. This extra cellular enzyme has been isolated using an engineered vector, purified to homogeneity and characterized. Optimization of the assay from lab level to plate level is in progress. A whole cell based assay for *Plasmodium falciparum HGPRT to be used for the screening of anti-malarial compounds has been developed on lab level.*

Digital information resource center

NCL has been in the forefront of deploying information technologies to help its scientists to be in the forefront in their chosen area of research. The information division contributes to the laboratory's success as a leader in R&D by bringing together information, knowledge, tools and systems for informed decision making for research and management. Towards this goal, the division has taken several strategic and timely initiatives in the field of information and communication technology.

Mission & goals

- Information and communication technology infrastructure development
- Digital library
- Tools and standards development for managing large data
- Business process support infrastructure
- Capacity building and HRD development
- R&D in scientific informatics

Competencies

- Chemoinformatics
- Biodiversity informatics
- Metadata and clearinghouse techniques development.
- Scientific database - data mining and knowledge management
- Web technology implementation

Infrastructure

- The DIRC facility provides for a centralized support for the information infrastructure. This includes an excellent campus wide local area network with about 700+ Computers, a range of servers, internet connectivity, access to a range of digital resources including databases like Chemical Abstracts, Current Contents, Chemical Business Newsbase on the intranet and online access to a large number of electronic journals (including back volumes for many) from leading publishers like Elsevier Science, American Chemical Society, Royal Society of Chemistry and Wiley Interscience.
- User room with a range of computers for easy and common access to digital information resources, productivity and other office tools, compute resources, visualization and modeling facility and access to special devices like scanners, CD writers etc.
- State-of-the-art classroom facility with PCs or workstations on each desk for human resources development and capacity building training.
- Server room with high performance servers managing centralized ICT services and information resources.
- Computer laboratory to set up experimental systems and test / evaluation platforms, softwares and applications.

The information division is actively involved in research and developments programs in "Scientific Informatics" primarily Chemical Informatics and Biodiversity Informatics.

Chemoinformatics

Variously known as chemoinformatics or cheminformatics, chemical informatics is the application of computer technology to chemistry in all of its manifestations. Massive amounts of physical and chemical property data are generated each year for new and existing chemical substances. Such an avalanche of data can bury a chemical research project unless ways can be found to cope with it. Chemical informatics can provide tools to acquire, organize, and evaluate data -- tools that yield new insights for further chemical research.

The focus of the Chemoinformatics group is in the areas of chemical synthesis planning, new chemical entities design, data analysis, data mining and data warehousing and QSAR. The group's interest also include Chemical warehouse databases systems with large set of chemical structures along with associated data are commonly used to centralize and secure chemical structures and related data. Such systems provide the features needed to centrally register and retrieve institutional such as experimental, computed and literature information. The web interface provides advanced fingerprint based search for exact-structure, sub-structure and similar-structure along with associated data. The research activities include:

- QSAR analysis of a) National Cancer Institute (NCI) Cancer dataset consisting in vitro screening of about 32000 open chemical structures for inhibitory activity of cell growth in the NCI 60 human cancer cell lines, b) NCI's database of about 42,000 molecules screened for anti AIDS activity and c) US-EPA's Fathead minnow (pimephales promelas) dataset: Distributed Structure searchable Toxicity data (DSSTox) using various computational tools like MOE, OELib etc., and algorithms and techniques like KNN, SVM etc.
- The Databases of chemical structures retrieved from private and public resources with drugs and drug likeliness molecules were analyzed for substructure, scaffolds and functional groups. The scaffolds derived from these datasets were further populated with additional functional groups to generate combi-libraries. These libraries of chemical structures were further analyzed by generation of molecular descriptors and screening algorithms for discovery drug like molecules. All the molecular data along with descriptor data, activity data were written as SDF (Standard data format) files to be exported to standard database tables like Oracle, MSSQL etc., where the scientific data can be further statistically analyzed for pattern and trend discovery.
- Additional efforts were made in mining chemical literature to identify molecules either synthesized or isolated at NCL or used for chemical research over last fifty years. . In this context a preliminary study on about 900 selected publications of NCL resulted about 12000

non-commercially available molecules with varying degree of novelty and complexity. This dataset will be analyzed and updated periodically along with associated information with unique identifier for building molecular registration system at NCL.

Biodiversity informatics

- **Electronic catalogue of known Indian fauna (IndFauna):** IndFauna currently disseminate baseline information on more than 60,000 of the known 90000 faunal species in India. IndFauna is accessible at http://www.ncbi.org.in/biota/fauna/.
- **Electronic catalogue of known Indian flora (IndFlora):** IndFlora currently disseminate baseline information on more than 14,000 of the known 45000 floral species in India. IndFlora is accessible at http://www.ncbi.org.in/biota/flora/
- **SAMPADA:** The Center has developed multi-taxon biological collections data management system called "SAMPADA". Its aim is to encourage curators and collections managers within India and in neighboring regions to automate the repository data and digitize the specimens. SAMPADA has been included in the list of recommended software's by GBIF and CODATA Taxonomic Database Working Group (TDWG).
- **ABCDIO:** Large numbers of our biological specimens are housed in the European and American museums. The center has developed web-based mechanism to "Access to Biological Collections Data of Indian Origin (ABCDIO)". As on date NCBI has been able to repatriate data on more than 30000 biological specimens housed in museums abroad. ABCDIO is accessible at http://www.ncbi.org.in/abcdio/.
- **Sacred groves information system:** The center is also developing ecosystems specific databases. We have initiated collaborative program with the Center for Development of Advanced Computing (C-DAC), Pune for developing Web GIS interfaced Sacred Groves Information System (SaGrIS). Currently, baseline data About sacred groves from Maharashtra, Andhra Pradesh, Tamil Nadu, and Karnataka can be accessed through our web portal at http://www.ncbi.org.in/.
- **Database on conservation sites:** The center is also working on development of "Database on Conservation Sites" which would collate information on national parks, wildlife sanctuaries, biosphere reserves, Ramsar sites, tiger reserves, botanical and zoological gardens, as well as community conserved areas.

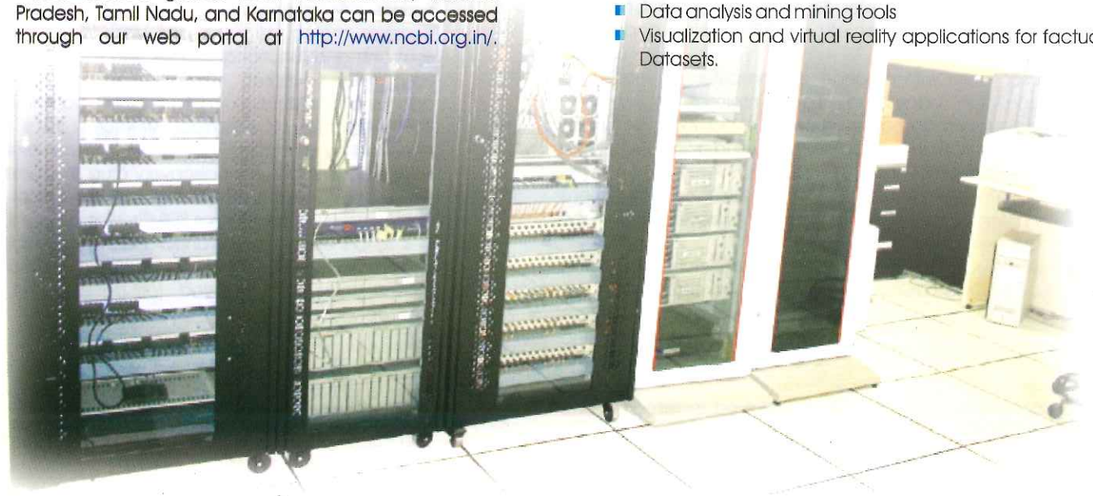
The center has also developed "Database of Indian Taxonomists (DIT)" which collates information about diverse taxonomic expertise available within the country. It also has web-interfaced databases on biological organizations within country and biological collections within South Asia. In addition to these information resources, a listserve (ncbi@listserve.ncl.res.in) to facilitate exchange/ sharing of ideas and views and also to provide platform for implementation of collaborative R&D ideas in the field of biodiversity informatics have been launched. The work program includes ensuring interoperability amongst datasets being developed in-house and those developed by the agencies within India and abroad.

Common threads

All the above-described programs have common threads or technical areas of work. Some of these are document management & workflows, metadata and clearinghouse techniques, digitization methods and standards, standardized terminology & controlled vocabulary, database, data mining and knowledge management techniques, web technology, and mobile and wireless computing.

Common activities will focus on

- Tools for harvesting information spread across the network and building up central depository
- Search and retrieval methodologies
- Digital Archival and Document Information Management System
- Design and Implementation of Electronic Lab Notebooks
- Data analysis and mining tools
- Visualization and virtual reality applications for factual Datasets.



National collection of industrial micro-organisms

NCIM is a pioneer microbial culture collection facility in India, which offers services to educational / research institutes and industries, besides various research programmes of NCL. NCIM is a unique resource dedicated to the isolation, collection, preservation and distribution of authentic cultures of industrially important microorganisms. NCIM holds about 3700 microbial strains of bacteria (1800), yeast (550), fungi (1300) and algae (15). The main objective of the facility is to supply authentic cultures to research institutes and industries. The catalogue of microbial strains can be accessed through http://www.ncl-india.org/nclindia/ncim.

Fermentor

Mission & goals

- Preservation of the microbial strains by a variety of Methods
- Distribution of authentic cultures to research institutes and industries
- Capacity building in culture collection
- Acting as repository of patent strains in addition to the strains used for basic research, indirectly helping to retain important microflora in the country
- Contract research and consultancy services

Competencies

- Isolation and preservation of microbial strains
- Strain improvement
- Microbial and biocatalytic processes for value added products
- Lyophilization of microbial cultures
- Long term preservation of specialized cultures Microbiological testing of samples

Infrastructure

- Fermentor (1 Lit 10 Lit)
- Bacterial lyophilizer
- Compound microscope with digital camera
- Inverted microscope
- HPLC
- GC

Bacterial lyophilizer

Glimpses of current research

Strain improvement for bio-ethanol production

Fungal strains were identified for cellulase production, which were further taken up for mutagenesis to obtain improved strain. The *Penicillium janthinellum* (NCIM 1169) was subjected to UV mutagenesis followed by EMS treatment, which resulted in the isolation of mutant strains capable of exhibiting bigger zones of hydrolysis of Walseth cellulose. These mutants were further studied in shake flasks for cellulase enzyme production. One of the mutants was found to produce enhanced levels of Fpase activity (3.2 IU/ml), CMCase (55 IU/ml), when grown in AMM medium containing 1 per cent CP-123.

Bioconversion of fusel oil for flavor production

The project deals with the identification of suitable commercial lipase or an organism capable of converting fusel oil to isoamyl acetate with higher efficiency. Out of three commercial preparations tested, *Candida antarctica* lipase was found to be converting isoamyl alcohol to isoamyl acetate within 4 hrs with approximately 80 per cent conversion efficiency. One of the fungal strains, *Aspergillus niger* (NCIM 1207) was also found to convert isoamyl alcohol to its acetate within 72 hrs with 70 per cent conversion efficiency. The optimization studies for the bioconversion are in progress.

Bioconversion are in progress.screening of marine acinetobacter sp. for production of biosurfactants

The project involves the isolation, identification of *Acinetobacter* strains from marine environment. Samples from marine environment were collected and attempts were made to get colonies on media selective for *Acinetobacter* cultures. More than one hundred colonies, which were further taken for identification studies have been isolated. Ten colonies as belonging to genus *Acinetobacter* based on morphological, biochemical and genetic transformation methods have been identified. These strains will be further characterized genetically and evaluated for bio-surfactant production.

Structural & functional mimicry of bio-systems-carbohydrates-laced synthetic polymers as microorganism nutrient source

Standardization of CO_2 evolution experiments from polymers is in progress. The growth experiments in shake flasks using bacterial/ fungal cultures for microbial attack on synthesized polymers are also being performed.

S & T SUPPORT SERVICES

ANNUAL REPORT 2003-2004

Business development

Since a significant portion of NCL's budget is generated through coniract R&D services, consultancy and technology licensing the laboratory has a separate Business Development Division (BDD) involved with various aspects of business planning, contracts management, strategy consulting, intellectual property and event management. The division is staffed with engineers and management graduates who work as technology facilitators interfacing with scientists, industries, government, financial institutions and other statutory agencies.

Business facilitation

NCL is constantly exploring opportunities to work with industrial customers on challenging research problems which have an impact on their performance. NCL realizes that it is the industrial customer that keeps research relevant to and focused on real world problems and opportunities. Great emphasis is placed, therefore, on understanding customer's needs, clearly defining deliverables and meeting customer's expectations.

The BDD undertakes a mapping of skill sets and patent portfolio available at NCL and contacts industrial customers relevant under the context. It then plays a technology facilitation role through discussions related to project proposals, pricing issues and contracts management. NCL believes in the credo that NCL wins only if its customer wins. Consequently, NCL constantly aims at building a win-win relationship with all its customers.

Public relations & events management

The Public Relations and Events Management group is involved with internal and external communications that support the NCL's business objectives and undertakes other public relations activity that effectively builds up the image of the organization at large. The group manages the interests of NCL in industry trade shows, exhibitions, conferences and other public forums and also has the responsibility of managing all press communications and media relations, besides organizing and implementing CSIR programme on CPYLS in Maharashtra.

Exhibitions: This year, the group organized NCL exhibition at India International Trade Fair (IITF, 2003) in CII-TEDO technology trade pavilion (New Delhi, 14-27 November, 2003) and CSIR exhibition at PharmaExpo 2003 (Chennai, 19-20 December, 2003).

Symposium / Seminar: The group coordinated INSA Annual General Meeting, XXXIII National Symposium in Crystallography, CSIR Annual Business Meet and InnoCentive Annual Conference

Special talk/ memorial lectures: The group coordinated CSIR Foundation day, NCL Foundation Day, National Science Day, Memorial lectures in the memory of former NCL Directors and special invited talks.

Intellectual property management

The IPR unit looks after the protection of Intellectual Property Rights mainly prosecuting and securing patents for inventions in NCL. The unit is involved with scrutinizing the drafts submitted by scientists, finalizing the complete specifications and coordination with the Intellectual Property Management Division of CSIR. 104 Foreign and 60 Indian patent applications were processed in addition to the ongoing work of the patent applications from the previous years.

IPR unit in collaboration with IPMD also oversees filing and securing patents in foreign countries including United States, Europe and other countries covered under Patent Cooperation Treaty.

Customer satisfaction index

CSIR, the parent body of NCL, has launched an independent unit called the "Customer Satisfaction and Evaluation Unit" (CSEU) that monitors the levels of satisfaction of our clients with R & D services that the CSIR laboratories offer.

Customers were asked to grade the laboratory on the following parameters with respect to the project that they had undertaken with NCL on a defined scale.

- **Objective :** To check if the broad direction of the achievements intended at the start were accomplished or not
- **Schedule :** To ascertain if work is accomplished, as per the time schedule committed at the start
- **Output :** To ascertain how much of the minimum tangible which is of value to the customer, has been as committed at the start
- **Usability :** To ensure that the customer is able to readily use the output without further processing and with prolonged Impact

CSEU has compiled the grades received into a Grade Point Average known as the Customer Satisfaction Index (CSI) score. The interpretation of CSI scores is as given below:

(i)	1.00 = CSI	Customer is highly dissatisfied
(ii)	1.00 < CSI < 3.00	Customer is not satisfied
(iii)	3.00 < CSI < 3.60	Customer is merely satisfied
(iv)	3.60 < CSI < 4.00	Customer is probably delighted

The latest CSI score available is for the year 2002-03. NCL is one of the seven laboratories that are categorized in chemical sciences group amongst CSIR labs. The average CSI for chemical sciences is 3.35. NCL's CSI for the last three years is as follows:

Year	CSI
2000-2001	3.184
2001-2002	2.950
2002-2003	3.175

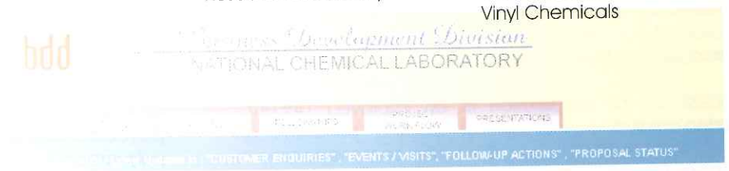
NCL's customers

GLOBAL

- ArQule
- Du Pont
- FDC
- Geltax Pharmaceuticals
- General Electric
- International Atomic Energy Agency
- Lyondell
- Millenium Research Lab
- National Research Council of Canada
- Proctor & Gamble
- Schenectady Specialities Asia
- Swiss Contact - IT Power Pvt. Ltd.
- UNICEF
- Unilever

INDIAN

Aarati Industries
Advanced Biochemicals
Amphenol International India
Aquapharm Chemicals
Asian Paints
Aspentech India
Astron Engineers India
Atul
Aventis CropScience India
AVRA labs
Bayer India
Bio-D Plastics
Chembiotek Research
CIPLA
Coffee Board
Central Pollution Control Board
D & O Pharmachem India
DGP Hinoday Industries
Directorate of Horticulture
Dura-line India
East India Pharmaceuticals
Emcure
Engineers India Ltd.
FMC India
Gas Authority of India Ltd
Garware Elastomerics
Garware Polyster
Glenmark Pharmaceutical Ltd.
Grasim Industries
Gujarat state Fertilizers and Chemicals
Heavy Water Board
High Energy Materials Research Laboratory
HLRC
ICI India
Indian Centre for Plastics in the Environment
Indian Seamless Steel & Alloys
Jubilant Organosys
Kirloskar Oil Engines Limited
Lupin Laboratories
Lupin Research Park
MedGene Biotech
Meghmani Organics
Ministry of Environment & Forests
Modepro India Pvt.Ltd.
Narmada Chematur Petrochemical
Navin Fluorine
Orchid Chemicals & Pharmaceutical
Pidilite Industries
Ranbaxy Laboratories
Reliance Industries
RPG Life Sciences Limited
S C Enviro agro India
Scope Pvt. Ltd
SJS Plastiblends
Smruti Organics
Specs and Biospecs
SRF
Sudarshan Chemical Industries
Tata Chemicals
Tonira Pharma
USV
Vikas Technologies
Vinati Organics
Vinyl Chemicals



Unencumbered patents (Indian)

Title of the invention	Patent number
A composition useful for the propagation of phragmites species	186894
A new enantioselective resolution process for arylpropionic acid drugs from the racemic mixture	189741
A new process for the preparation of uniform ultrathin films of metal oxide, metal chalcogenides or metal halides	189191
A process for enhancing cell-bound penicillin acylase activity through permeabilization and subsequent stabilization with a crosslinking reagent	182405
A process for reforming of pyrolysis naphtha	175609
A process for the catalytic conversion of methane or natural gas to syn gas	188329
A process for the hydrodewaxing of petroleum oils for the production of dewaxed oil	175147
A process for the oxidative conversion of ethane or C2-C4 paraffins to ethylene and higher olefins using the improved supported catalyst	188871
A process for the preparation of 5,6- didehyro 5-methyl PGFα2 derivative	185790
A process for the preparation of 7[1-(alkoxy carbonyl) propyl 5,6,7,8,9,11- hexahydro-8- (alkoxy carbonyl) indolizino [1,2b] quinolin-9-one	186969
A process for the preparation of a novel porous crystalline material vanadiam silicate, VS-2	184236
A process for the preparation of a soluble homogeneous catalyst useful for the preparation high molecular weight narrow molecular weight distribution of non crystalline polymers of α -olefins containing at least four carbon atoms	186303
A process for the preparation of an improved supported catalyst	189145
A process for the preparation of an improved supported catalyst useful for the oxidative coupling of methane to higher hydrocarbons, oxidative conversion of natural gas to ethylene and other lower olefins etc	188538
A process for the preparation of ceramic-polymer composite materials and components	189146
A process for the preparation of compounds bearing urethane linkage useful as plasticizer for polyvinylchloride (PVC)	188825

Title of the invention	Patent number
A process for the preparation of crystalline metallo titanium, catalyst composite material	183415
A process for the preparation of crystalline sodium alumino silicate	188874
A process for the preparation of crystalline vanadium titanium silicate	180196
A process for the preparation of e(-) silane, {[1- (2-iodoethenyl) -1- methylhexyl] oxy}trimethyl	185389
A process for the preparation of estra-5a- hydroxy -a-en- 11b- [4-(2-methyl-1,3-dioxolyl) phenyl] -17b-hydroxy -17a- (3-methyl-1- butynyl) -cyclic -3- (1,2,-ethandiyl) acetal	186134
A process for the preparation of extracellular arabinose liberating exo-xylanase from a pure yeast strain	182604
A process for the preparation of hydrolytically stable macroporous beads	182590
A process for the preparation of improved compounded polyvinylchloride (PVC)	188046
A process for the preparation of metal-polymer composite materials and components	188894
A process for the preparation of micro mesoporous amorphous titanium silicates	189703
A process for the preparation of microporous crystalline molybdenum silicate molecular sieves	187347
A process for the preparation of misoprostol	184735
A process for the preparation of monochlorophthalic anhydride free from dichloro component	188690
A process for the preparation of novel bioxyanion catalysts useful for the preparation of polycarbonates and a process for the preparation of polycarbonates using the said catalysts	177237
A process for the preparation of novel composite catalysts useful for oxidative conversion of methane (or natural gas) to carbon monoxide and hydrogen (or synthesis gas) in presence of free oxygen	184285
A process for the preparation of novel crystalline borosilicate	184408
A process for the preparation of novel macroporous glycidyl copolymers based beads useful as matrix for anchoring hydrophobic biomolecules	187419

Title of the invention	Patent number
A process for the preparation of novel macroporous spherical beads of glycidyl copolymers	184871
A process for the preparation of novel protease tolerant to high pH, high temperature and high levels of chromium ions	186995
A process for the preparation of optically active carboprost methyl ester	186339
A process for the preparation of poly (aryl ester carbonate)s	186156
A process for the preparation of poly (aryl ester-carbonate)s	186155
A process for the preparation of products crystalline molybdate tin-containing molecular sieve	189460
A process for the preparation of semipermeable membranes from silicon containing aromatic polyesters	186839
A process for the preparation of supported bimetallic catalyst useful for the hydrogenation of dicarboxylic acid esters	185715
A process for the production of 1-chloro-naphthalene	189203
A process for the production of a novel porous crystalline tin-containing molecular sieve	189306
A process for the production of linear alkylbenzenes	181008
A process for the recovery of purified thiocarbamide	184739
A useful process for the preparation of ankle block component useful for artificial foot	187915
An enzymatic process for the preparation of optically pure isomers of ethyl 2,3-dihydroxy -3- (4-methoxyphenyl) propanoate	185277
An improved composition useful for promoting development of shoots from the excised embryoaxes of cotton	189032
An improved naphtha reforming process for the preparation of a mixture of hydrocarbon rich in aromatics	187354
An improved process for catalytic hydroformylation of alkenes	188332
An improved process for selective hydrogenation of esters dicarboxylic acid	185714
An improved process for the continuous production of cheese	186454

Title of the invention	Patent number
An improved process for the conversion of alcohol to mixture of olefins	184107
An improved process for the conversion of methanol to olefinic hydrocarbons	178460
An improved process for the conversion of phenol to hydroquinone and catechol	189405
An improved process for the conversion of poly ethylene terephthalate (PET) waste to poly (alkyleine terephthalate) useful as an engineering thermoplastic	187889
An improved process for the manufacture of crystalline alumino silicate designated as ZSM-	176176
An improved process for the oxidation of olefinic organic compounds	186074
An improved process for the oxidative halogenation of aromatic compounds	186078
An improved process for the preparation of (1R,cis) - (-)- caronaldehydic acid hemiacetal	188978
An improved process for the preparation of (2R,3R)- methyl-phenyl glycidate	186876
An improved process for the preparation of aromatic aldehydes	189161
An improved process for the preparation of caprolactam from cyclohexanone oxime using micellar solution, macroemulsion and micro emulsion systems	189045
An improved process for the preparation of copper catalyst supported on a metal oxide	189479
An improved process for the preparation of cumene	177993
An improved process for the preparation of cyclopropylamine	184740
An improved process for the preparation of dihydroxybenzenes and 1,4-benzoquinone by the hydroxylation of phenol using titanium containing zeolite catalyst	179730
An improved process for the preparation of dihydroxybenzone, 1,4-benzoquinone by the hydroxylation of phenol using hydrogen peroxide and titanium containing zeolites	177718
An improved process for the preparation of ethanol	187087
An improved process for the preparation of formaldehyde using improved iron molybdate catalyst	185627

Title of the invention	Patent number
An improved process for the preparation of halocumenes	188375
An improved process for the preparation of high molecular weight narrow molecular weight distribution non crystalline hydrocarbon soluble polyolefins	185719
An improved process for the preparation of hydroxy compounds of steroids	185379
An improved process for the preparation of iron molybdate catalyst	185935
An improved process for the preparation of mono-alkyl carbonate of bisphenols	185382
An improved process for the preparation of n-acetyl aminophenol	189140
An improved process for the preparation of novel cross linked mesoporous crosslinked glycidyl methacrylate - penta erythritol triacrylate copolymers	186430
An improved process for the preparation of novel crosslinked macroporous of lycidyl methacrylate - divinyl benzene copolymers	187315
An improved process for the preparation of optically active carboprost methyl ester	185768
An improved process for the preparation of phenol hydroxybenzene and 1,4-benzoquinone by hydroxylation of benzene using titanium containing synthetic zeolite catalyst	179711
An improved process for the preparation of phenol, dihydroxy benzenes, 1,4-benzoquinone by hydroxylation of benzene	179729
An improved process for the preparation of phenol, dihydroxybenzenes and 1,4-benzoquinone simultaneously by hydroxylation of benzene using phase transfer catalyst	184725
An improved process for the preparation of poly (arylester-carbonate)s	186146
An improved process for the preparation of polymeric device with uniform controlled porosity and containing one or more active ingredients	189033
An improved process for the preparation of porous crystalline silicate TS-	175810
An improved process for the preparation of substituted acetophenones	185806
An improved process for the preparation of titanium silicates	189381
An improved process for the preparation of unsaturated hydroxy lactones	189048
An improved process for the preparation of α-bromophenylacetic acid	190435

Title of the invention	Patent number
An improved process for the preparation of α cyclodextrin glycosyl transferase enzyme	188412
An improved process for the production of alcohol particularly ethanol	185720
An improved process for the production of cumene	176692
An improved process for the production of cycle oils having lower pour points	176724
An improved process for the production of cyclohexanone and cyclohexanol	178378
An improved process for the production of cyclohexanone and cyclohexanol	179085
An improved process for the production of ethylene by non-catalytic oxidative cracking of ethane or ethane rich C2-C4 paraffins	188334
An improved process for the production of immobilised d-amino acid oxidase	186455
An improved process for the production of immobilization milk clotting protease	187316
An improved process for the production of synthesis gas by oxidative conversion of methane using composite catalyst containing transitional and alkaline earth metal oxides	184286
An improved process for the production of the 1,1',1" - tris (4'- hydroxyphenyl) ethane	187237
An improved process for the selective oxidation of hydrocarbons and their derivatives	190356
An improved process for the separation of dihydroxy benzene isomers from aqueous phase using super absorbent polymers	177118
An improved process for the simultaneous preparation of 1,4 benzoquinone and hydroquinone	184488
An improved process for thermostabilizing α-l-arabinofuranosidase enzyme	186723
An invention relates to a process for the preparation of an alkaline protease from an alkalophilic streptomycete in semisolid fermentation	189297
Energy efficient process for the oxidative conversion of methane or natural gas to ethylene, ethane and higher hydrocarbons using the improved supported catalyst	188872
Improved process for making high quality steel directly from fine particles of iron rich materials and non cocking coal fines	176146
Process for the preparation of crystalline titanium silicate TS-2	175727
Process for the preparation of hydrophilic stable macro-porous beads	189324

Unencumbered patents (Foreign)

Title of the invention	Patent number
(2R,3S,22R,23R)-2,3,22,23-Tetrahydroxy-24-ethyl-β-homo-7-oxa-5α-cholestan-6-one and a process for preparing the same	6090952
1,3-Oxazoline compounds useful as anionic initiators suitable for polymerization of vinyl polymers	5266702
A new polymer composition	5780578
A new process for the preparation of uniform ultrathin films of metal oxide, metal chalcogenides or metal halides	5549931
A new strain of cephalosporium having accession no. ATCC 74292, a process of isolating said strain of cephalosporium and a process for preparing extracellular endoxylanase	5534429
A novel catalyst composition material and a process for the preparation of a novel catalyst composite material	135159
A process for the preparation of an imported supported catalyst useful for the oxidative coupling of methane to high hydrocarbons, oxidative conversion of natural gas to ethylene and other lower olefins and oxidative dehydrogenation of lower alkanes	5712217
A process for the preparation of (2R,3S,24S)-2,3-diacetoxy-22-bromo-24-ethyl -β- homo -7-oxa -23-hydroxy -5α-cholestan -6-one	6008380
A process for the preparation of a magnesium halide supported metallocene catalyst	5962360
A process for the preparation of a new polymer useful for drag reduction in hydrocarbon fluids in exceptionally dilute polymer solutions	0471116
A process for the preparation of a new polymer useful for drag reduction in hydrocarbon fluids in exceptionally dilute polymer solutions	2023298
A process for the preparation of adipic acid	0784045
A process for the preparation of αand β naphthol by hydroxylation of naphthalene using an organotransition metal complex	0867424
A process for the preparation of an active composition containing triterpenes including azadirachtin and its derivatives possessing insect antifeedant and growth inhibitory activity from parts of the neem plant	5602261
A process for the preparation of an improved supported catalyst	5744419

Title of the invention	Patent number
A process for the preparation of caprolactum	5401843
A process for the preparation of new reactive anionic initiators useful for polymerization of vinyl monomers	0477444
A process for the preparation of novel composite catalysts useful for oxidative conversion of methane or natural gas to synthesis gas	0582004
A process for the preparation of poly (ester-carbonate)s	908483
A process for the preparation of silicon containing polyarytates	5820992
A process for the preparation of supported bimetallic catalyst useful for the hydrogenation of esters of dicarboxylic acids	5792875
A process for the preparation of supported metallocene catalyst	5965477
A process for the production of p-dialkyl benzene	135162
A process for the production of polyhydroxyoctanoate by streptomyces lividans	6692945
A process for the selective oxidation of hydrocarbons and their derivatives	5811599
Alkalothermophilic bacillus that produces a protease inhibitor	6448060
An improved catalyst useful for the preparation of carboxylic acids	2999597
An improved catalyst useful for the preparation of carboxylic acids	1974954
An improved catalyst useful for the preparation of carboxylic acids	8803781
An improved integrated two step process for conversion of methane to liquid hydrocarbons of gasoline range	5336825
An improved process for catalytic hydroformylation of alkenes	5498801
An improved process for preparing of α & β naphthol	5932732
An improved process for the conversion natural gas into middle distillates	621640
An improved process for the conversion of lower alkane(s) to aromatics or higher hydrocarbons under non-oxidative conditions and low temperature	5936135
An improved process for the conversion of natural gas into middle distillate	246301

Title of the invention	Patent number
An improved process for the preparation of alkyl carbamates	0442173
An improved process for the preparation of alkyl carbamates	5502241
An improved process for the preparation of aromatic polyesters	0807655
An improved process for the preparation of caprolactam from cyclohexanone oxime using micellar solution, macroemulsion and microemulsion systems	5594137
An improved process for the preparation of halocumenes	5892138
An improved process for the preparation of high molecular weight poly (aryl carbonates)	0568740
An improved process for the preparation of methyl ethyl ketone secondary butyl alcohol using an improved copper silica catalyst	5723679
An improved process for the preparation of mixture of guaiacol and p-methoxy ethanol	5786519
An improved process for the preparation of n-acetyl aminophenol	5856575
An improved process for the preparation of thioanides from carboxylic acids	5510490
An improved process for the preparation of titanium silicates	5885546
An improved process for the single step oxidation of 3-phenoxy tolunene to 3-phenoxybenzaldehyde	5693869
An improved process for the synthesis of d (+) biotin	0564723
An improved reforming process for the catalytic conversion of petroleum fractions to a mixture of hydrocarbons rich in aromatics	0382960
Bromo - functionalised benzotriazole UV absorbers	6284895
Catalyst composite material for hydrocarbon reactions	0474928
Catalyst composite material for hydrocarbon reactions	2025449
Catalyst composite material for hydrocarbon reactions	22474
Catalyst composite material for hydrocarbon reactions	5141908
Catalyst composite material for hydrocarbon reactions	625926

Title of the invention	Patent number
Catalyst system containing a semilabile anionic ligand and a use of such catalyst system to produce α, β, -unsaturated carboxylic acids and their esters	6331502
Catalytic reforming process utilizing an iron-and lanthaum-containing metallosilcate zeolite	5262045
Composition for hybrid seed production, process for the preparation of such composition and use thereof	6645917 B2
Compound bearing an urethane linkage, which is an addict of ricinoleic esters and an isocyanate, useful as a plasticizer for polyvinyl chloride (PVC) and a process for preparing such compound	6437032
Cultural medium for bamboo shoot sprouting and multiplication and a method for sprouting and multiplication of bamboo plantlets	5750401
Culture medium composition useful for induction and proliferation of Taxus calli	6365407
Diol - functionalized UV absorber	6307055
Enantioselective resolution process for arylpropionic acid drugs from the racemic mixture	6093830
Halophilic pseudomonas strain having accession no.ncim 5109 (ATCC 55940) and a process for preparation d(-)n-carbamoylphenylglycine using said strain	6121024
Hydrophobic composite Pd-membrane catalyst useful for non-hazardous direct oxidation of hydrogen by oxygen to hydrogen peroxide and method of its preparation	6448199
Hydrophobic multicomponent catalyst useful for direct oxidation of hydrogen to hydrogen peroxide	6346228
Improved process for the preparation of codeine from morphine	0268710
Lanthanum silicate catalyst composite, its preparation and its use for conversion of alkanols to light olefins	1277650
Low temperature process for the production of hydrogen	6509000
Macromonomer	0982334
Membrane process for the production of hydrogen peroxide by non-hazardous direct oxidation of hydrogen by oxygen using a novel hydrophobic composite Pd-membrane catalyst	6432376
Method and an apparatus for the identification and or separation of complex composite signals into its deterministic and noisy components	6208951

Title of the invention	Patent number
Microbial process for the production of d(-)-n-carbamoylphenylglycine	6087136
Microbial process for the production of d(-)-n-carbamoylphenylglycine	6280979
Microencapsulation of monocrotophos	5962003
Micro-meso amorphous titanium silicate catalyst	5795555
Mifepristone analogue, process for the preparation thereof and use thereof	6512130
N-1-alkyl-2,5-di(trialkyl silyl) pyrrolidines	5654439
Nickel containing catalyst	0352378
Noble metal containing hydrogenation catalyst for selective hydrogenation of 1,4-butynediol to 1,4 butenediol, and a process for the preparation thereof	6660675
Noble metal containing hydrogenation catalyst for selective hydrogenation of 1,4-butynediol to 1,4-butenediol, and a process for the preparation thereof	6528689
Novel composite catalysts containing transitional and alkaline earth metal oxides useful for oxidative conversion of methane (or natural gas) to carbon monoxide and hydrogen (or synthesis gas)	5756421
Novel compound having urethane linkage, which is an adduct of ricinoleic esters and an isocynate, useful as a plasticizer for polyvinyl chloride (PVC) and a process for preparing such compound	5952411
Novel compound having urethane linkage, which is an adduct of ricinoleic esters and an isocynate, useful as a plasticizer for polyvinyl chloride (PVC) and a process for preparing such compound	6118012
Novel triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity and a process for extracting such compounds from the neem plant	5395951
Novel triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity and a process for extracting such compounds from the neem plant	5663374
Novel triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity and a process for extracting such compounds from the neem plant	5756773
One pot method for preparation of 1-[2-dimethylamino -(4-methoxyphenyl) - ethyl] cyclohexanol	6350912

Title of the invention	Patent number
Pesticidal ester preparation	5750757
Polyimides, process for the preparation thereof and use thereof as alignment films for liquid crystal devices	6500913
Polymer composition for controlled release of active ingredients in response to pH, and a process of preparing the same	5851546
Preparation of ethanol using supplements	6015699
Preparation of improved nickel-containing catalyst and process for the conversion of alcohols to carboxylic acids therewith	4902659
Preparation of polyurethane microspheres by non aqueous dispersion polymerisation	5859075
Process and production ethylene by non-catalytic oxidative cracking of ethane or ethane rich C2-C4 paraffins	5763725
Process for catalytic hydrogenation of organic compounds	5650546
Process for making alkyl n-alkyl or n-aryl-thiocarbamates	5621132
Process for making s(-) amlodipine salts	6608206
Process for oxidative conversion	6087545
Process for polymerization of olefins	6187882
Process for preparation of 2-phenyl ethanol	6166269
Process for preparation of a lactone from a cyclic ketone	6559322
Process for preparation of carboxylic acid and their esters	6294687
Process for preparation of semisynthetic amplicons useful for determination of sex in papaya	6037128
Process for preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst	6525226
Process for preparing enantiomerically pure (s)-3-hydroxy-γ-butyrolactone	6713639
Process for preparing of diltiazem	6180785
Process for producing alcohol	5455163
Process for producing polycondensable macromonomer	6022930

Title of the invention	Patent number
Process for production of propylene and ethylene by non-catalytic oxycracking of propane or propane-rich C2-C4 paraffins	6020534
Process for production of synthesis gas by oxidative conversion of methane or natural gas using composite catalysts	5368835
Process for simultaneous preparation of sex specific and gender - neutral semisynthetic amplicons useful for sex determination	6180345
Process for synthesis of d(+) biotin	5274107
Process for the activation of a metallic palladium based catalyst useful for the direct oxidation of hydrogen to hydrogen peroxide	6534440
Process for the activation of pervoskite type oxide	6197719
Process for the acylation of aromatic compounds using a reusable solid catalyst comprising indium halide	6437191
Process for the catalytic conversion of methane or natural gas to syngas or a mixture of carbon monoxide and hydrogen	6293979
Process for the conversion of 1,4-butynediol to 1,4-butanediol, or a mixture of 1,4-butenediol and 1,4-butanediol	6469221
Process for the conversion of 1,4 butynediol to 1,4 butenediol	6420615
Process for the conversion of natural gas into middle distillates	1325814
Process for the conversion of phenol to hydroquinone and catechol	5493061
Process for the conversion of polyethylene terephthalate waste to poly alkaline terephthalate	5451611
Process for the liquid phase acylation of aromatic compounds	6459000
Process for the oxidation of cyclohexane to a mixture of cyclohexanone and cyclohexanol	5767320
Process for the oxidation of cyclohexane to adipic acid	6392093
Process for the photochemical production of α aryl propionic acid	4906343
Process for the photochemical production of α-aryl propionic acid	2565977
Process for the preparation of (4R,6S)-4-hydroxy-6-hydroxymethyl-tetrahydropyran-2-one	6376683

Title of the invention	Patent number
Process for the preparation of β hydroxy-ä lactone using novel intermediates	6388097
Process for the preparation of 1-[cyano(aryl)methyl] cyclohexanol	6504044
Process for the preparation of 2-acrylamido-2-methyl-1-propanesulfonic acid	6504050
Process for the preparation of 2-aryl propionic acids	6660883
Process for the preparation of 2-methyl-2-propene-1-sulfonic acid, sodium salt	6660882
Process for the preparation of 4(r)-hydroxy cyclopent-2-en1(s)-acetate	6448051
Process for the preparation of 5-methoxy-4(methylthioalkyl)-1,3-bis(phenyl methyl)-2 imidazolidinone useful as an intermediate for the d(+) biotin synthesis	6350881
Process for the preparation of a carboxylic acid	6444844
Process for the preparation of a carboxylic acid	6380426
Process for the preparation of a magnesium halide supported metallocene catalyst	5955554
Process for the preparation of a mixture of 19 hydroxyeicosatetraenoic acid and 20 hydroxyeicosatetraenoic acid (19 HETE and 20 HETE)	6379937
Process for the preparation of a nanosized colloidal metal particle	6537344
Process for the preparation of a new polymer useful for drag reduction in hydrocarbon fluids in exceptionally dilute polymer solutions	5080121
Process for the preparation of a polyesteramide	6410681
Process for the preparation of acetic acid or methyl acetate	6521784
Process for the preparation of acidic lipase	6534303
Process for the preparation of adipic acid	6521789
Process for the preparation of alkyl 4[2-(phthalimido)ethoxy]-acetoacetate	6562983
Process for the preparation of an improved Li-promoted MgO catalyst useful for oxidative coupling of methane to ethane and ethylene	5118654
Process for the preparation of aqueous urethane dispersions	6239213
Process for the preparation of aralkylated aromatic compounds using heterogeneous catalyst	6215035

Title of the invention	Patent number
Process for the preparation of aromatic polyesters	5714567
Process for the preparation of aromatic polyesters	6420511
Process for the preparation of aryl esters of n alkyl carbonic acids	0446514
Process for the preparation of aryl esters of n-alkyl carbonic acids	5066819
Process for the preparation of β- hydroxy-δ lactone using novel intermediates	6417374
Process for the preparation of bromo - functionalized benzotriazole UV absorbers	6320056
Process for the preparation of catalyst composite material designated encilite	129327
Process for the preparation of codeine from morphine	4764615
Process for the preparation of diesters of poly(oxyalkylene glycol) and amino acids	6346643
Process for the preparation of dihydroxydiphenylmethanes	6492566
Process for the preparation of enzymatically degradable polymers	6316585
Process for the preparation of ibuprofen	6093847
Process for the preparation of lithium stanates doped with transition metal cations	5461013
Process for the preparation of molecularly imprinted polymers useful for separation of enzymes	6379599
Process for the preparation of mono-alkylcarbonate of bisphenols	5627301
Process for the preparation of nanodimensional particles of oxides and sulphides of metals	5643508
Process for the preparation of new transition metal complexes	6069253
Process for the preparation of nitrile group containing polymers	5194537
Process for the preparation of novel molecular sieves	5219813
Process for the preparation of novel vinylic hindered amine light stabilizers	6489482
Process for the preparation of n-substituted acrylamides	6369249
Process for the preparation of phenyl ketones	6593499

Title of the invention	Patent number
Process for the preparation of polyesters	6335415
Process for the preparation of polyurethane microspheres	5814675
Process for the preparation of polyurethane spherical particle	6123988
Process for the preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst	6548722
Process for the preparation of thermoprecipitating affinity polymers	6420487
Process for the preparation of thermoprecipitating affinity polymers	6689836
Process for the preparation of thiourea	6657082
Process for the production of aromatic carboxylic acids	6649791
Process for the production of linear alkyl benzene	0564724
Process for the production of linear alkylbenzenes	5453553
Process for the production of synthesis gas by oxidative conversion of methane (or natural gas) using composite catalyst containing transitional and alkine earth metal oxides	5338488
Process for the recovery of potassium bitartarate and other products from tamarind pulp	6316615
Process for the recovery of tartaric acid and other products from tamarind pulp	5994533
Process for the selective esterification of tertiary alcohol by an acid anhydride using a reusable solid catalyst	6420596
Process for the synthesis of a photo-stabilizer	6559311
Process for the trans-esterification of keto esters using solid acids as catalysts	6376701
Process for treatment of mixture of spent wash from distillery and black liquor from pulp and paper industry	6589427
Process of preparing composite catalysts for production of synthesis gas by oxidative conversion of methane or natural gas	5411927
Reforming process for the catalytic conversion of petroleum fractions to a mixture of hydrocarbons rich in aromatics	4950385
Single step hydrogenation of nitrobenzene to p-aminophenol	6403833

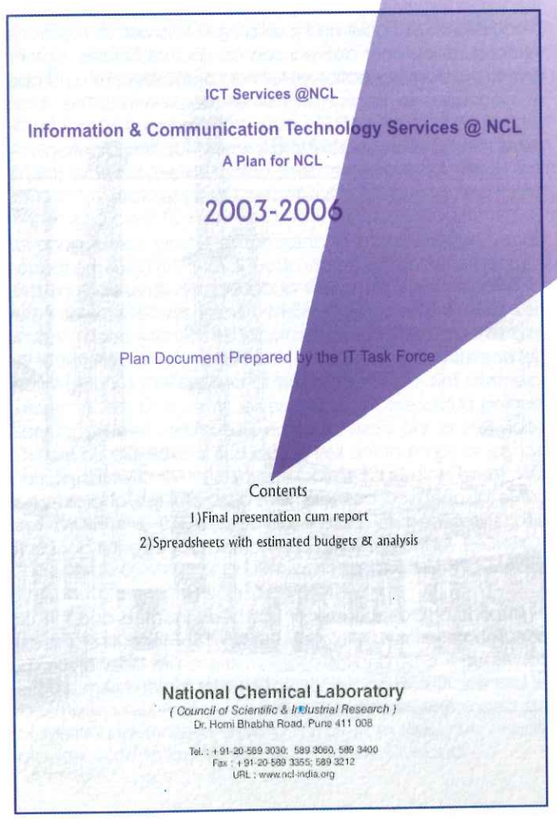
Title of the invention	Patent number
Single step process for the preparation of p-aminophenol	6028227
Single step process for the preparation of poly(oxyalkylene)-α,ω -dicarboxylic acid	6239252
Strain of streptomyces for the preparation of an alkaline protease inhibitor	6514748
Substituted 2-[-6-benzyl-5-oxo-3-phenyl-(3s,7s,7ar)-perhydroimidazol[1,5-c][1,3]thiazol-7yl] compounds	6486328
Supported catalyst useful for Friedel - Crafts reaction and process for the preparation of aralkylated aromatic compounds using the catalyst	6180557
Thermoprecipitating polymer containing enzyme specific ligands, process for the preparation thereof, and use thereof for the separation of enzymes	6605714

Title of the invention	Patent number
Tinuvin p-hindred amine light stabilizer and derivatives thereof	6492518
Tinuvin p-hindred amine light stabilizer and derivatives thereof	6610856 B2
Triterpene derivatives of azadirachtin having insect antifeedant and growth inhibitory activity and a process for extracting such compounds from the neem plant	5663374
Two step process for production of liquid hydrocarbons from natural gas	5306854
Water soluble palladium complexes and process for the preparation thereof	6469169

Information division

Information division

The Information Division (ID) has the responsibility to design and manage the information infrastructure for the laboratory. The division is continuing to make effective use of Information technology (IT) to provide the intellectual infrastructure in terms of access to a wide range of Information resources located within NCL as well as in outside world, to enable the scientists of NCL to perform better and to maintain its leadership position. Besides, the division has initiated work on Chemical Informatics and Biodiversity Informatics. The laboratory had set up IT Task Force to visualize, anticipate and define NCL's future (short term and long term) needs in terms of all information resources, services, systems and infrastructure (scientific, institutional, management and administrative) while keeping in view the emerging trends in information and communication technology, information system and business management, scientific and technical information resources etc.


ICT Services @NCL

Information & Communication Technology Services @ NCL

A Plan for NCL

2003-2006

Plan Document Prepared by the IT Task Force

Contents

1)Final presentation cum report

2)Spreadsheets with estimated budgets & analysis

National Chemical Laboratory

(Council of Scientific & Industrial Research)

Dr. Homi Bhabha Road, Pune 411 008

Tel. : +91-20-589 3030; 589 3060, 589 3400
Fax : +91-20-589 3355; 589 3212
URL : www.ncl-india.org

IT Vision of NCL

- Digitization of all laboratory processes both on scientific and operational sides - by 2010.
- World-class Information and Communication Technology (ICT) systems and infrastructure so as to make possible continuously increasing levels of operational efficiency, convenience, speed & security, informed management decisions and effective leadership. Aim to be global benchmark for effective and intelligent deployment and use of ICT systems, services and infrastructure for research laboratories by 2013.
- World-class national resource center for scientific information relevant to the chemical sciences, allied disciplines and related industries by 2005.
- Global resource center for the research, conception and early-stage development of high-end IT-driven knowledge-based solutions, services and products relevant to the chemical sciences, allied disciplines and related industries by 2010.
- Immediate and easy access to/ availability of world-class scientific computing resources for research and design by NCL scientists by 2005.

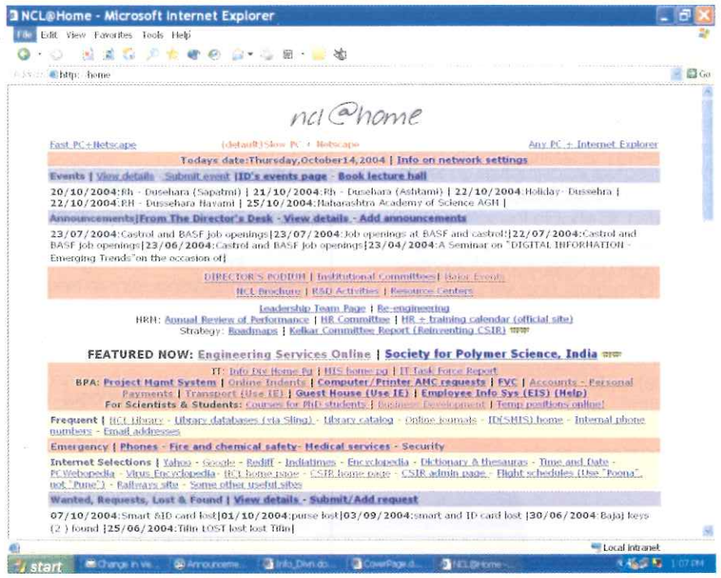
ICT Systems

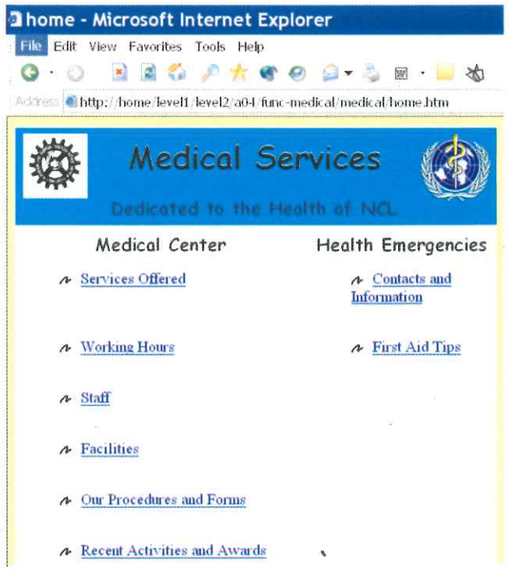
NCL has been in the forefront of deploying information technologies to help its scientists to excel in their chosen area of research. NCL has an excellent campus wide local area network (LAN) with about 700 computers, a range of servers to host databases, e-mails systems, web services and a good connectivity to the internet. The ICT plan of the laboratory is closely dovetailed to the IT vision of NCL. Some of the highlights of this year are:

- High speed core switch to support gigabit speeds
- Upgraded some of the links to gigabit
- Security devices like Firewall, IDS in place
- Centralized caching engine
- Long Range Ethernet for access from remote sites
- Centralized antivirus system
- New website www.ncl-india.org

For transparent access to information NCL has local home page called NCL@HOME for campus wide information dissemination. NCL Staff Recreation Club conducted its annual elections online successfully. It has the pages for:

- Director's podium
- Finance & Accounts
- Staff welfare club
- Resources for employees
- Students & career
- NCL alumni association
- Medical services





Library & information services

The basic functions of library and information service include procurement of books and journals (print as well as electronic versions), document delivery service (journal articles, patents and standards), translation of technical articles from a number of languages to English and other user services. The library subscribes to around 250 journals (200 Foreign & 50 Indian), 30 series titles, and procures approximately 400 books annually. All the library functions are done using Library software (LIBSYS) which has resulted in fast & effective Library services.

Library has launched an informative Library home page on intranet furnishing the details about library. This helps the readers to access the information about library services from their desktops. This includes Current Awareness Service of newly added journals & books in the library. Efforts have been made to get access to a large body of information on the desk top of the scientists. This includes access to a number of journals from leading publishers like ACS, Elsevier, Wiley and RSC (including back files in the case of some publishers). Besides journals, access to some of the key databases is available on the NCL LAN. These include Chemical Abstracts (1977 onwards), current contents, chemical business news base etc. The laboratory has also subscribed to patent databases like DELPHION, and SCIFINDER. All these efforts have helped NCL scientist access to a library at their desktop.

Digitization of old documents has been initiated and the old documents (print & microfiche) from 1868 and onwards are converted into CD and the printed material has been preserved as archive. Till now about 300 volumes of major Chemistry titles has been converted into CD form.

Management information system

MIS Group handles all activities related to Project Management System. The activities can be broadly classified as follows:

- Assistance to scientists in preparation of project Proposals as per CSIR guidelines.
- Coding of New projects and preparation of new project Initiation note for circulation to all concerned departments.
- Allocation of funds to the projects and circulation of challan to all concerned.
- Preparation and raising of invoices for Industrial Projects
- Extension of projects in consultation with scientists.
- Issuing of completion Certificate of Projects.
- Calculation and payment of service tax for consultancy and technical services projects to Central Excise Department.
- Maintenance of service tax records as per CSIR guidelines for consultancy and technical services projects.
- Providing audit information on NCL projects.
- Laboratory budget preparation/ allocation / monitoring
- Preparation of financial and performance reports of NCL.
- Developing appropriate systems for MIS functions
- Providing Information on projects to MC/RC Meetings.
- Management of NCL Research Foundation and its activities
- General assistance in the management and smooth functioning of the Laboratory.

Efforts are being made continuously to streamline the procedures relating to project initiation, monitoring and closure. Many of the activities have been computerized. There is an efficient system to track the receipt of funds for various projects, monitoring cash flows, project monitoring, publication profiles etc.

A web enabled project management information systems was developed in-house to support the activities of the group. This system takes care of the financial aspects (receipts, budgeting) of projects from initiation to completion. It stores all the important information about the project:

- Project Information
- Funds receipt
- Party Information
- Staff deployed
- Project Installments

The systems provides for generating a range of reports to enable the management to review the status.

The MIS portal offers access window to PMIS for the scientific staff, project leader, HOD's and management teams. The site offers hierarchical login to different users. This enables to control the information depending on the requirements of the user and prevents unauthorized viewing. Apart from PMIS, the site also provides information on NCL performance, Divisional performance, various proforma for downloading, about NCL research foundation activities etc. This portal will be the driving force for providing financial information to NCL Scientists.

Document management system

NCL, at any time, has about 300 internal and external projects running throughout the year. The turnover from externally funded projects is about Rs.15 Crores and Rs. 10 Crores is from internal CSIR funded projects. Therefore it becomes a monumental task to maintain project records and answer queries from Project leaders and government auditors. In order to ensure smooth functioning of Project Management and maintenance of project records, MIS Group developed internally a Project Management Information System (PMIS) to take care of Project documentation at NCL.

PMIS is a centralized document management system holding all project records at one place. The project records are available to the concerned scientists through MIS website (24 x 7 hours). MIS group creates all the project records internally and same is made available on the MIS website to the scientists. The scientists are provided with a login and password to access their project records directly from their desktops. All project documents like agreement, project proposal, project initiation, challans, funds received and due are available on the fly as and when the records are created by MIS group. In addition, there is an upload facility for scientists to upload interim and final reports submitted to the client and project output summary into the PMIS system. Therefore all financial and scientific reports are centralized and stored in MIS server and all project records can be created as when required.

PMIS creates important reports for management for decision making. The External cash flow reports, Lab reserve earnings, detailed project break up, dollar earnings, funds due from project are some of the important management reports available to HOD's and Director. In addition, queries can be created to pull out information from the database as and when required. PMIS sends alert mails, whenever a payment is due. This helps MIS group to raise invoice and collect the funds in time. The alert mail is also send to the scientists, whenever a report to the client is due and scales up the alerts to HOD and Director, if the request is not complied.

Human resource management

Human Resource Management Unit focuses on the training needs of the laboratory for both scientific and support staff. The unit has the following responsibilities:

- Drawing up of a training calendar for the year
- Preparing budget estimates for training needs
- Identifying the faculty as well as designing the contents of the training programmes
- Organization of the training programmes
- Creating a mechanism of collecting feedback from participants and analysis thereof
- Placing proposals before Director, NCL with specific suggestions as well as nominations for deputing personnel for training outside NCL

Following training programmes were organized by the unit:

Training imparted to NCL staff

- **Training programme on materials management :** To upgrade technical and non-technical skills of the employees and expose them to up-to-date modern trends in their respective fields a three-day programme in Materials Management was organized for the staff members of the Stores & Purchase Section. This programme in two batches was conducted by NITIE, Mumbai.

- **Training programme on patents and regulatory issues:** It has become imperative for the scientists involved in drug development research to know patents and related issue. For scientists engaged in the research problems related to Drug / Pharmaceuticals industry, a two-day training programme on "Patents & Regulatory Issues in Pharmaceutical Industry" was conducted by National Academy of Legal Studies & Research(NALSAR), University of Law, Hyderabad.

- **Training programme for Canteen and Guesthouse personnel:** The training programme was conducted by "The Maharashtra State Institute of Hotel Management and Catering Technology", Pune. To identify the areas where the training would be needed, the faculty members of the institute visited both the Canteen and the Guesthouse. The institute covered the areas like food production, food and beverage service, institutional house keeping and front desk operations (reception) and training for control (supervisors). Twenty NCL employees attended the training from one week to one month in two batches related to the area of their functioning.

Training imparted to outsiders

- NCL conducted a three-day training course on **"Rheology of Polymeric and Complex Fluids"** for the employees of GE-WTC, Bangalore covering the lectures, data interpretation sessions, hands-on lab sessions and course notes The course was especially designed for the participants of GE-WTC to provide training in the fundamentals of the science of rheology and its implications in elucidating structure-property relations in polymeric and complex fluids.

- A school on **"Modeling and Optimization for Performance Enhancement in Process Engineering"** was organized during January 19 to 22, 2004 at NCL to make use of the strong expertise available at the Chemical Engineering Division of NCL in the areas of process modeling, simulation and optimization. About 30 participants from universities, R& D institutions and industry attended the school.

DST-SERC

- **HIDECOR training programme :** The rationale for the Human and Institutional Development in Ecological Refrigeration (HIDECOR) project (2001-04) is phasing-out Chlorofluorocarbon (CFC) from Refrigeration and Air-conditioning (RAC) servicing sector to comply with the phase out targets under the Montreal Protocol (MP). The HIDECOR project operates within the larger policy framework set by the MP. Indian RAC sector consumes significant amount of CFCs. Indian refrigeration service sector consists of about 40,000 enterprises and about 77,000 technicians. It is important for technicians to know safe and good servicing practices with alternative refrigerants as these refrigerants are not as friendly as earlier (CFC) refrigerant was. Therefore, the sector plan was prepared with significant direct input from various stakeholders including industry, refrigeration associations, service enterprise owners and academic and R&D institutions (NCL and IIT, Delhi).

Under HIDECOR project high quality and user friendly programmes are designed for such technicians. Training material and programme is standardization by NCL and IIT Delhi. A network is established in 11 states for conducting these programs and recruiting deserving participants. These programs are sponsored by Swiss Agency for Development and Cooperation (SDC), New Delhi and organized by Swisscontact IT Power India Pvt. Ltd. (SC-ITPI) Consortium at Pondichery. The program target is to train about 10,000 technicians by end of 2004; of which 7,300 are already trained till 2003. The training programs are conducted at three levels viz. for Engineering College Professors (AR&C), Training for Trainers (TOT), and for Micro and Small Enterprise Technicians (MSET). So far, 10 ARACs (3 day program), 5 TOTs (5 day programs) and about 400 MSETs have been conducted in the select states.

NCL is actively involved in these training programmes. Equipments required for good servicing practices were provided to NCL by HIDECOR such as Evacuation and Charging, Recovery and Recycling alternative refrigerants to CFC and lubricating oil. NCL is also actively involved in indigenous development of recovery and recycling unit for the benefit of Indian technicians. So far 4 AR&C programs were coordinated by NCL at IIT Bombay, IIT Kharagpur and Anna University. NCL has also conducted / participated in several TOTs and monitored many MSETs (about 50) programmes.

This year, about 165 MSE training programs were conducted in the selected states, training about 3350 technicians. Also during this period, 2 TOT programs and 4 PTAC programs were conducted.

Research fellows & project assistants

NCL's intake of Research Fellows who qualify in CSIR NET examination is around 350 at any point of time. Thus, NCL is responsible in contributing 40-50 Ph.D. holders each year. Govt. funded institutions and private bodies enter into agreements with NCL under sponsored/ consultancy projects programme. It is extremely difficult to undertake these projects with the existing manpower and as such engage persons exclusively for the work relating to projects, which is co-terminus with the duration of the project, to assist the scientists in achieving the target set for completion of the project. Normally around 375 Project Assistants are in NCL at any point of time. The experience gained by them in such positions is a step for better employment opportunity in the open market.

Apprentice scheme

The Apprentice Act is applicable to NCL/ CSIR and accordingly around 25 positions of Apprentices are filled up each year in different trades such as Electronics Mechanical, Refrigeration & A/C Mechanics, Instrument Mechanics, Mason, Plumber, Carpenter, Fitter, Turner, Welder etc. The Apprentices deputed to NCL are students pursuing their studies at ITI institutions in and around the State of Maharashtra and this apprenticeship at NCL is a part of the curriculum for ITI courses. The experience gained by them at this level is of immense value for their future career.

PhD Degrees (2003)

Author	Title	University	Guide
Ali, I.S.	Asymmetric synthesis of bioactive molecules using asymmetric hydrosylation, aziridination of olefins and kinetic resolution of alcohols	Pune	Sudalai, A.
Ashavani Kumar	On the problems related to hydrophobization and assembly of inorganic nanoparticles	Pune	Sastry, M.
Badarayani,R.D.	Effect of ionic solutes on amino acids and peptides from thermodynamic, volumetric and transport studies: experiments and correlations	Pune	Anil Kumar
Barve, M. (Ms.)	Insight into genomic architecture of fusarium oxysporum f. Sp. Ciceri and ascochyta rabiei the two major fungal pathogens of chickpea (cicer arietinum l.)	Pune	Gupta, V.S. (Ms.)
Bennur, T.H.	Selective oxidations and carbon-carbon bond forming reactions using transition metal catalysts	Pune	Sivasanker, S.
Bhattacharya, A.	Stereoselective synthesis of alpha-hydroxy acid derivatives and studies on the synthesis of ethophenprox	Pune	Pansare, S.V.
Cherian, J.	Synthetic studies toward mycolactones, eupomatilone-8 and some novel compounds	Pune	Gurjar, M.K.
Dewkar, G. K.	Asymmetric synthesis of bioactive molecules and synthetic methods involving oxidation of n-h, o-h bonds and oxidative halogenation of arenes and alkenes	Pune	Sudalai, A.
Gaikwad, B.G.	Studies on the production, extraction, purification and use of hydantoinase	Pune	Kulkarni, B.D.
Galgali, G.	Synthesis structure processing property relationships in polymer nanocomposites	Pune	Lele, A.
Gogate, S.S. (Ms)	Studies on in vitro morphogenetic response of horticultural crop-cashew	Pune	Nadgauda, R.S.
Joseph, T.	Synthesis, characterisation and catalytic properties of intra-zeolite transition metal complexes	Pune	Gopinathan, S.
Khandare, J. K.	Studies on affinity precipitation of biomolecules using stimuli sensitive polymers	Mumbai	Kulkarni, M.G.

Author	Title	University	Guide
Krishnaswamy, D.	Stereocontrolled synthesis of substituted azetidin-2-ones	Pune	Deshmukh, A.R.A.S.
Mandal, D.	Fungal mediated biotransformations of organic (carbonyl group) and inorganic compounds	Pune	Rajiv Kumar
Mukhopadhyay,K.	Studies on heterogenization of metal complex catalysts by encapsulation in zeolites and mesoporous materials	Pune	Chaudhari, R.V.
Pandey, R.K.	Asymmetric dihydroxylation and wittig-horner approach to the synthesis of bioactive molecules and heterogeneous catalysis for organic transformations	Pune	Pradeep Kumar
Ramachander, T.V.N.	Characterization of a 5.0 kb genomic dna fragment from streptomyces aureofaciens nrrl 2209 involved in polyhydroxybutyrate (PHB) synthesis	Pune	Rawal, S.K.
Sandhya, T.E.	Synthesis and characterization of aliphatic aromatic polyesters	Pune	Sivaram, S.
Shaikh,N.S.	Organic chemical transformations using a) palladium and b) clay as catalysts	Pune	Deshpande, V.H.
Shyamroy, S.	Synthesis of biodegradable poly(lactic acid) polymers	Pune	Sivaram, S.
Singru, R.S.	Molecular characterization of genetic variation in s. graminicola and understanding host pathogen interaction	Pune	Ranjekar, P.K.
Soni, P.B. (Ms)	Synthetic studies towards biotin and development of useful synthetic methodologies	Pune	Chavan, S.P.
Suresh Kumar, T.	Stereoselective functionalizations on arene chromium template	Pune	Sarkar, A.

NCL Scientists recognized by different universities as research guides

Name	University
Dr. Anil Kumar	Pune
Dr. Argade, N.P.	Pune, Mumbai
Dr. Bakre, P.P.	Pune
Dr. Bastawde, K.B.	Pune, Shivaji University, Kolhapur
Dr. Bhadbhade, M.M.	Pune
Dr. Chanda, (Mrs) Bhanu	Pune
Dr. Chandwadkar, (Ms) A.J.	Pune
Dr. Chaudhari, R.V.	Pune, Mumbai, Shivaji University, Kolhapur
Dr. Chavan, S.P.	Pune
Dr. Chumbhale, V.R.	Swami Ramanand Teerth Marathwada University, Nanded
Dr. Deshmukh, A.R.A.S.	Pune
Dr. Deshpande, (Mrs) Vasanti	Pune
Dr. Deshpande, M.V.	Pune, North Maharashtra University, Jalgaon, Shivaji University, Kolhapur
Dr. Deshpande, R.M.	Pune
Dr. Dongare, M.K.	Pune, Mumbai
Dr. Ganapathy, S.	Pune
Dr. Ganesh, K.N.	Pune
Dr. Garnaik, (Ms.) B.	Pune
Dr. Gokhale, D.V.	Pune, Shivaji University, Kolhapur
Dr. Gopinath, C.S.	Pune
Dr. Gupta, (Mrs) Vidya	Pune
Dr. Gupte, S.P.	Pune
Dr. Gurjar, M.K.	Pune, Mumbai, Osmania University, Hyderabad
Dr. Guruswamy, K	Pune, IIT Mumbai
Dr. Halligudi, S.B.	Pune, Bhavnagar
Dr. Hegde, S.G.	Swami Ramanand Teerth Marathwada University, Nanded
Dr. Jaganathan, R.	Pune
Dr. Jayaraman, V.K.	Pune
Dr. Jog, (Mrs) J.P.	Pune, Shivaji University Kolhapur
Dr. Joshi, (Mrs) S.P.	Pune
Dr. Joshi, N.N.	Pune
Dr. Joshi, P.N.	Swami Ramanand Teerth Marathwada University, Nanded
Dr. Joy, P.A.	Pune
Dr. Kalkote, U.R.	Pune
Dr. Kelkar, A.A.	Pune
Dr. Khan, M.I.	Pune, North Maharashtra University, Jalgaon
Dr. Khire, J.M.	Pune
Dr. Krishnan, S.	Pune
Dr. Kulkarni, B.D.	Pune, Mumbai, Nagpur, Shivaji University, Kolhapur
Dr. Kulkarni, M.G.	Pune, Mumbai
Dr. Kulkarni, R.A.	Pune
Dr. Kumar, (Mrs) V.A.	Pune
Dr. Lachke, Anil	Pune
Dr. Lele, A.K.	Pune, Mumbai
Dr. Manikandan, P.	Pune
Dr. Mayadevi, (Mrs) S.	Pune

Name	University
Dr. Mukherjee, S.N.	Pune
Dr. Mulla, I.S.	Pune
Dr. Nadgauda, (Mrs) Rajani	Pune
Dr. Natarajan, Upendra	IIT Mumbai
Dr. Natu, A.A.	Pune, Shivaji University, Kolhapur
Dr. Pal, Sourav	Pune
Dr. Pandey, Ganesh	Pune, Osmania University, Hyderabad, Shivaji University, Kolhapur
Dr. Pedireddi, V.R.	Pune
Dr. Ponrathnam, S.	Pune
Dr. Pore, (Mrs) V.S.	Pune
Dr. Prabhune, (Mrs) Asmita	Pune
Dr. Prasad, S.D.	Pune
Dr. Pundle, (Ms) Archana	Pune
Dr. Puranik, (Mrs) V.G.	Pune
Dr. Radhakrishnan, S.	Pune
Dr. RajaMohanan, P.R.	Pune
Dr. Rajiv Kumar	Pune
Dr. Ramaswamy, (Mrs) Veda	Pune
Dr. Ramesh, C.	Pune
Dr. Ranade, V.V.	Pune, Mumbai
Dr. Rao, (Mrs) Mala	Pune, Shivaji University, Kolhapur
Dr. Ravi, V.	Pune
Dr. Rele, (Mrs) M.V.	Pune
Dr. Rode, C.V.	Pune
Dr. Rojatkar, S.R.	Pune
Dr. Sainkar, S.R.	Pune
Dr. Sanjayan, G.J.	Pune
Dr. Sastry, Murali	Pune
Dr. Satyanarayana, C.V.V.	Pune
Dr. Seetalaxman, (Mrs) R.	Pune
Dr. Shankar, V.	Pune
Dr. Shashidhar, M.S.	Pune
Dr. Singh, A.P.	Pune
Dr. Singh, R.P.	Pune
Dr. Sivaram, S.	Pune, Mumbai, IIT Mumbai
Dr. Sivasanker, S.	Pune, Shivaji University, Kolhapur
Dr. Srinivas, D.	Pune, Bhavnagar
Dr. Srinivasan, K.V.	Pune
Dr. Sudalai, A.	Pune
Dr. Suresh, C.G.	Pune
Dr. Tare, (Mrs) V.S.	Shivaji University, Kolhapur, Yashwantrao Chavan Maharashtra Open University, Nashik
Dr. Tewari, R.	Pune
Dr. Tripathi, P.K.	Pune
Dr. Varma, A.J.	Pune
Dr. Vijayamohanan, K.	Pune
Dr. Wadgaonkar, P.P.	Pune
Dr. Wakharkar, (Mrs) R.D.	Pune

Publication and science communication

The unit manages i) content for NCL website and intranet, ii) press releases, iii) digitisation of archives, iv) publication v) science communication aspects of laboratory and vi) liaison with CSIR.

Website: The NCL website was completely revamped and launched. The content is continuously being updated by the unit. The unit also interacted with web developer on various aspects of designing and development of website.

Press releases: The unit releases press notes on all important occasions and events. It communicates important R&D reports for publication in CSIR News and CSIR Samachar. The unit also attends to press enquiries.

Digitisation of archives: The unit has started digitisation of all important records of historical value which are in various formats like text, photographs, audio and video cassettes.

Publication: The unit is entrusted with the publication of annual report of NCL. The unit provided NCL inputs for CSIR annual report 2002-03 and 2003-04. It also provided inputs for "CSIR status on rural technology".

Liaison with CSIR: The unit attended to various queries of CSIR Hq related to information dissemination.

Research planning and audit

Research Planning & Audit Unit was involved in areas of research planning, staff deployment, budget, project monitoring, and liaison with CSIR. The unit liaises with CSIR in providing research utilization data of NCL on a quarterly basis. It co-ordinated with project leaders, finance and purchase officials and Director and provided outputs on patents and major achievements in basic and applied science, besides highlighting the work done and funds generated through technology services.

The unit interacted with CSIR on queries raised in C&AG Audit report. The unit has also interfaced with the audit party from the Principal Director of Audit, Scientific Department (Mumbai) on matters related to projects and satisfied the queries.

The unit conducted review meetings to monitor in-house projects (4), major mission mode projects (2), co-ordination of Network projects (X plan) (2), NMITLI projects () and projects under X Five Year Plan (). The unit arranged and organized two Research Council meetings of NCL. It also organized an internal training course for senior scientists for the newly introduced Annual Review of Performance (ARP) system. The unit also prepared a database on the technology developed and licensed by NCL during last 50 years.

Safety management

The health and safety of all staff is of paramount importance to NCL. The Standing Committee on Laboratory safety involving member representation from all the divisions was reconstituted in April 2003. In addition, divisional safety committees were also constituted with member representation from scientific staff and research students. The standing committee meets regularly at an interval of three months and reviews overall safety in the laboratory. Safety committee has organized four meetings and the divisional sub-committees have organized two meetings each. The central committee and divisional sub-committees also carried out three inspections in each division. Safety action plan has also been devised with many new initiatives. This included:

- Periodic Fire fighting training programs including mock drills to all scientists, students, and project staff,
- Manual fire alarm system in all laboratories,
- Design and creation of a fire safe solvent storage area for bulk solvents,
- Inventory of large volume solvent storage in each laboratory,
- Defining norms of persons per square meter laboratory space,
- Explore cost benefit of insurance cover for all expensive equipment, and
- Review of electrical safety hazards

Restricted use of carcinogenic & highly toxic chemicals

Selected 30 chemicals, which have been classified as "known carcinogens" to humans are notified and their procurement, use, storage and disposal is restricted. The use of mercury and benzene is also being completely stopped to make the campus free from mercury and benzene. Digital gauges are being used to replace mercury vacuum gauges.

Solvent storage facility

A safe solvent storage facility has been formulated. For better and safe distribution of solvents, two air-operated diaphragm pumps with clutch operated dispensing nozzles have been installed for the delivery of solvents.

Fire safety

Three fire safety training programmes have been conducted with the aid of external experts. More than 300 staff and research students have availed of the training. Seventy fire extinguishers have been installed in various parts of the laboratory to strengthen fire fighting abilities. About eighty sand/ fire buckets have been installed in all the wet chemical laboratories.

Eyewash fountains

Eyewash fountain and safety showers in practically every wet chemistry laboratory have been provided. Twenty-two eyewash fountains have been installed in organic chemistry laboratories totalling the number of eyewash fountains installed to forty.

National Safety Day was observed on 10th March 2004. As a part of this event various programmes like fire-fighting demonstration, presentation of a safety plan by Chairman, Safety Committee and film-shows on Chemical & Fire Safety were organized. Safety representatives presented the highlights of the work done in their respective divisions. Dr. T. Rajgopalan, Chief Medical Officer, Hindustan Lever Limited delivered the lecture on "on "Occupational Health and Safety in Chemical Laboratories" on Safety Day.

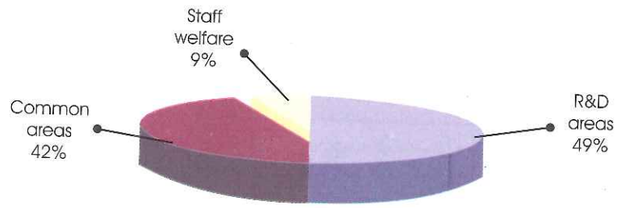
Dr. T. Rajgopalan, Chief Medical Officer, Hindustan Lever Limited, Mumbai delivering lecture on Occupational Health and Safety in Chemical Laboratories

Engineering services

Engineering Services Unit (ESU), comprising mechanical, electrical and civil engineering sections, looks after overall maintenance and renovation of existing facilities and creation of new facilities. The unit has in-house design and drawing (CAD) facility. This year a new building was constructed in the campus at a total cost of Rs 1.4 Crores for Digital Information Resource Center (DIRC) which added 7800 sq.ft. of office space. Besides, conference hall in the main building, guest house rooms, Director's secretariat, Business Development Division and several laboratories were completely renovated. The unit has procured an ecofriendly battery operated platform truck for transportation of various types of material within the campus. This facility is operated by the staff themselves. The campus road leading to Baner Road from NCL colony was widened. ESU organized free service camp for repair of large number of vacuum pumps and also trained two of its technicians at the company workshop in maintenance.

Many of the research programmes at NCL require the fabrication of state-of-the-art equipments. The workshop undertook fabrication of sample holder for rheometer, gas permeation cell, gas cylinder adopters as well as installation and commissioning of steam explosion digester. Continuous support for the modification of reformer for hydrogen generation was provided.

The ESU handled work and services worth Rs 4.45 Crores during the year 2003-04. The distribution of activities was as under:



Break-up of Works & Services expenditure for 2003-04 in terms of end users

Director's secretariat

Conference Hall

Meeting Room

Digital Information Resource Center

Renovated Laboratories

प्रशासन विभाग

प्रशासन विभाग ने संगठन की कार्यक्षमता को बढ़ाने तथा वैज्ञानिक स्टाफ द्वारा किए जा रहे अनुसंधान कार्य में तत्काल सहायता प्रदान करने हेतु अनेक नए कदम उठाए हैं। इसके अन्तर्गत निम्नलिखित नए कार्य आरम्भ किए गए :

- प्रशासन की सभी गतिविधियों/कार्यों का उचित रूप से वर्गीकरण किया गया तथा कार्य के स्वरूप के अनुसार संबंधित कागजातों के निपटान हेतु न्यूनतम/अधिकतम समय निर्धारित किया गया। स्टाफ के सभी सदस्यों में इसका व्यापक प्रचार-प्रसार किया गया है। इसके कार्यान्वयन/अनुपालन की तिमाही रिपोर्ट निदेशक महोदय को प्रस्तुत की जाती है।
- अधिकारों के प्रत्यायोजन का पुनरीक्षण/समीक्षा की गई तथा जहाँ आवश्यक है वहाँ उसका स्पष्टीकरण प्रस्तुत किया गया और इसे स्टाफ में व्यापक स्तर पर परिचालित किया गया।
- प्रशासनिक कार्यों में सूचना प्रौद्योगिकी के अधिकाधिक प्रयोग को शुरू किया गया। अतिथिगृह के आरक्षण एवं स्टाफ कार के लिए माँगपत्र प्रस्तुत करने की ऑन-लाइन व्यवस्था की गई।
- कर्मचारियों की उपस्थिति दर्ज करने तथा कार्यालय भवन में प्रवेश हेतु स्मार्ट कार्ड आधारित प्रणाली लागू की गई।
- प्रत्येक कर्मचारी का सम्पूर्ण सूचना से युक्त एक समग्र डेटाबेस तैयार किया गया।

वित्त एवं लेखा

वित्त एवं लेखा अनुभाग में आरम्भ किए गए कार्य :

- सभी वाउचरों युक्त आकस्मिक बिलों की ऑन-लाइन प्रस्तुति।
- प्रत्येक कर्मचारी के बैंक खाते में जमा किए गए भुगतान के विवरण की ऑन-लाइन सूचना।
- इन्ट्रानेट पर प्रत्येक कर्मचारी के सामान्य भविष्य निधि खाते में मासिक शेष राशि की ऑन-लाइन सूचना।
- ग्राहक संतुष्टि मूल्यांकन यूनिट का अलग खाता खोलना एवं उसका रखरखाव
- 1628 लेखा आपत्तियों का समायोजन
- 2002-03 तक 66 में से 41 लेखापरीक्षा अनुच्छेदों का निपटारा

वर्ष 2003- 04 के दौरान बजट राशि की उपयोगिता

	रु. लाख में
एन.एम.आई.टी.एल.आई. व्यय	452.012
वापस की गई राशि	351.082
क्षतिपूर्ति व्यय	378.045
निवेश	800.000
सा.भ.नि./अं.भ.नि.	475.337
वैज्ञानिक पूल	4.834
वाहन/कम्प्यूटर अग्रिम	7.985
कुल	9284.608

वर्ष 2003- 04 के दौरान बनाए गए वाउचर

	संख्या
भुगतान	20,456
प्राप्ति	5,043
अन्तरण प्रविष्टि	770
पूंजी	13
बकाया	
आय	4
व्यय	151
कुल	26,437

भण्डार एवं क्रय

भण्डार एवं क्रय अनुभाग में आरम्भ किए गए कार्य :

- क्रय माँगपत्र की ऑन-लाइन प्रस्तुति।
- रु. दस हजार (10,000) तक की रेट-कॉन्ट्रैक्ट वाली मदों की माँगों पर ऑन-लाइन कार्रवाई और 48 घंटों के अन्दर उनकी आपूर्ति का आश्वासन।
- सामान्य स्टॉक में सभी प्रकार की लेखन सामग्री तथा कम्प्यूटर हेतु उपभोज्य वस्तुओं और अन्य सामग्री की उपलब्धता। भण्डार में कम से कम सामान रखने के प्रयास के अन्तर्गत केवल आवश्यक वस्तुओं की आपूर्ति।
- नकद खरीद के बिलों का उनकी प्रस्तुति के समय से 24 घंटों के अन्दर अधिप्रमाणन।
- नवम्बर, 2002 से एन.सी.एल. इन्ट्रानेट के माध्यम से ऑन-लाइन माँगपत्र प्रस्तुति का प्रारंभ।
- भण्डार एवं क्रय स्टाफ में बहुकार्य योजना का कार्यान्वयन, भण्डार एवं क्रय स्टाफ के एक दल की अनेक प्रकार के कार्यों में संलिप्तता।

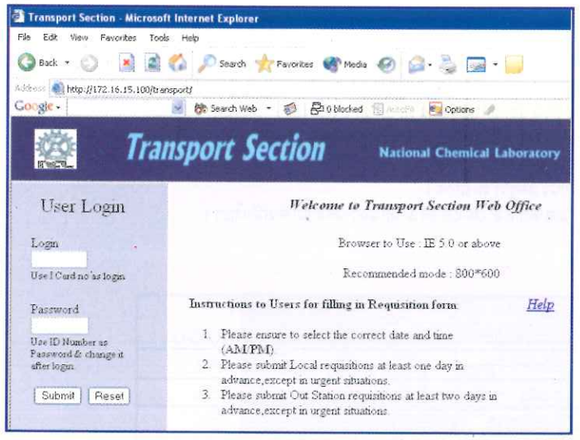
भण्डार एवं क्रय द्वारा सम्पादित कार्य

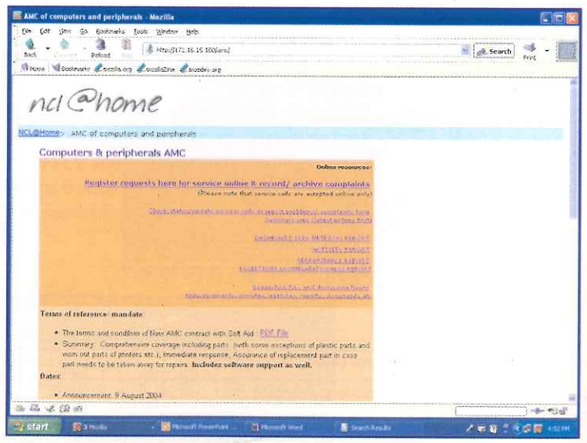
मद	संख्या		मूल्य (रु. करोड़ में)	
	2002-03	2003-04	2002-03	2003-04
कुल प्राप्त एवं निपटाए गए माँगपत्र	2256	2613	21.5	28.9
कुल दिए गए क्रयादेश (विदेशी)	406	653	16.5	18.6
कुल दिए गए क्रयादेश (देशी)	1686	6958	6.7	12.1
कुल प्राप्त सामग्री (विदेशी)	876	944	16.8	14.1
कुल प्राप्त सामग्री (स्वदेशी)	2580	2275	7.0	8.3
स्थानीय क्रय	7273	8521	1.2	2.0
भण्डार से दी गई कुल सामग्री	20831	21122	—	—

Administration

The Administration Department has taken several new initiatives to enhance the efficiency of the organisation and to provide prompt support to the scientific staff in pursuit of their endeavours. The following new initiatives were implemented:

- All activities of the administration were suitably categorized and minimum / maximum time for processing the papers were prescribed depending on the nature of activity. These were widely publicized to all staff. Quarterly compliance reports were made available to the Director.
- The delegation of powers were reexamined, clarified where necessary, and widely circulated amongst staff.
- Increasing applications of IT in administrative functions were introduced. Guest house bookings and staff car requisition were made online.
- Smart card based attendance marking as well as building entry system was made operational.
- A comprehensive employee database was created.





Finance and Accounts

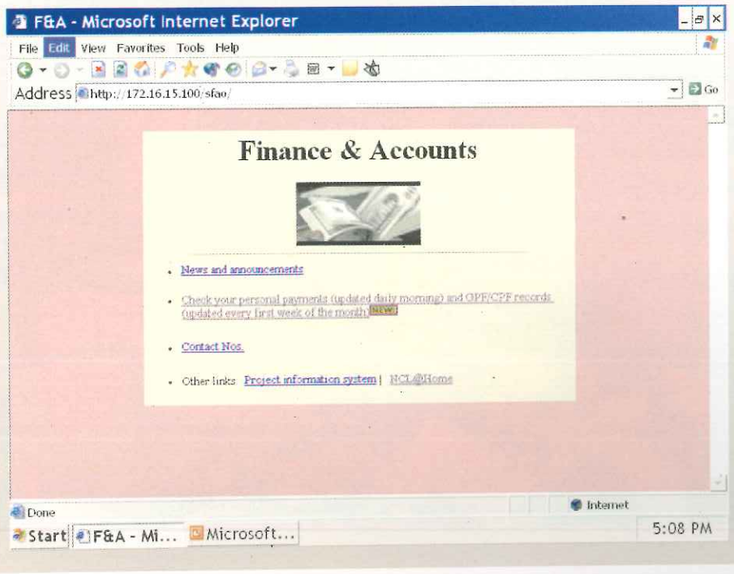
- Online submission of Fully Vouchered Contingent Bills
- Online information about the details of payments credited to the Bank account of each employee.
- Online monthly GPF balance of each employee on the intranet.
- Opening and maintenance of separate account of CSE Unit
- OB clearance : 1628
- Settlement of audit paras : 41 out of 66 up to 2002-03

Budget utilization during 2003-04

	Rs. in lakh
NMITLI Exp.	452.012
Remittance Expenditure	351.082
Recoupment Expenditure	378.045
Investment	800.000
GPF/ CPF	475.337
Sci. Pool	4.834
Conv. Adv./Computer Adv.	7.985
Total	9284.608

Vouchers created during 2003-04

	Nos.
Payment (P)	20,456
Receipt (R)	5,043
Transfer Entry (T/E)	770
Capital (C)	13
Outstanding:	
- Income	4
- Expenditure	151
Total :	26,437



Stores and Purchase

Initiatives adopted in Stores and Purchase

- Online submission of purchase indent
- Request for Rate Contract items up to Rs. 10,000/- being processed online with assured delivery to Scientist's desk within forty eight hours
- All stationary as well as consumables for PCs and peripherals available in general stock
  Steps taken to minimize stores inventory to essentials
- Cash purchase bills certified within twenty four hours of receipt
- Online indenting system operational since November 2002 through the NCL intranet system
- Multitasking amongst Stores and Purchase staff implemented; A team of Stores and Purchase staff handle a basket of Services

Stores and Purchase: Accomplishments

Item	Numbers		Value (Rs. In crores)	
	2002-03	2003-04	2002-03	2003-04
Total indents received and processed	2256	2613	21.5	28.9
Total orders placed (imported)	406	653	16.5	18.6
Total orders placed (indigenous)	1686	6958	6.7	12.1
Total consignment received (imported)	876	944	16.8	14.1
Total consignment received (indigenous)	2580	2275	7.0	8.3
Local purchases	7273	8521	1.2	2.0
Total Stores issues	20831	21122	—	—

APPENDIX

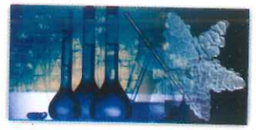
ANNUAL REPORT 2003-2004

Top papers published (2003)

Title / author	Journal affiliation	IF
Regioselective protection and deprotection of inositol hydroxyl groups: Sureshan, K.M.; Shashidhar, M.S.; Praveen, T.; Das, T.	Chemical Reviews, 2003, 103(11), 4477	21.036
Terpenoid Metabolism in Wild-Type and Transgenic Arabidopsis Plants. Aharoni, A.; Giri, A.P.; Deuerlein, S.; Griepink, F.; Kogel, W.; Verstappen, F.W.A.; Verhoeven, H.A.; Jongsma, M.A.; Schwab, W.; Bouwmeester, H.J.	The Plant cell, 2003, 15(12), 2866	10.679
Single-strand-specific nucleases: Desai, N.A.; Shankar, V.	FEMS Microbiol Reviews, 2003, 26(5), 457	10.160
Strategic developments in living anionic-polymerization of Alkyl(methyl) acrylates: Baskaran, D.	Progress in Polymer Science, 2003 28(4), 521	7.759
Room-temperature synthesis of aragonite crystals at an expanding liquid-liquid interface in a radial Hele-Shaw cell: Rautaray, D.; Banpurkar, A.; Sainkar, S.R.; Limaye, A.V.; Pavaskar, N.R.; Ogale, S.B.; Sastry, M.	Advanced Materials, 2003, 15(15), 1273	7.305
Keggin Ions as UV-Switchable Reducing Agents in the Synthesis of Au Core-Ag Shell Nanoparticles: Mandal, S.; Selvakannan, P.R.; Pasricha, R.; Sastry, M.	J American Chemical Society, 2003, 125(28), 8440	6.516
Biosynthesis of $CaCO_3$ crystals of complex morphology using a fungus and an actinomycete: Rautaray, D.; Ahmad, A.; Sastry, M.	J American Chemical Society, 2003, 125(48), 14656	6.516
Slow tight binding inhibition of proteinase K by a proteinaceous inhibitor - Conformational alterations responsible for conferring irreversibility to the enzyme- inhibitor complex: Pandhare, J.; Dash, C.; Rao, M.; Deshpande, V.	J Biological Chemistry, 2003, 278(49), 48735	6.482
Essential polyunsaturated fatty-acid and lipid peroxide levels in never-medicated and medicated schizophrenia patients: Arvindakhan, M.; Sitasawad, S.; Debsikdar, V.; Ghate, M.; Evans, D.; Horrobin, D.F.; Bennett, C.; Ranjekar, P.K.; Mahadik, S.P.,	Biological Psychiatry, 2003 53(1), 56	6.039
Aspartic peptidase inhibitors: Implications in drug Development: Dash, C.; Kulkarni, A.; Dunn, B.; Rao, M.	Critical Reviews in Biochemistry & Molecular Biology, 2003, 38(2), 89	5.318
Highly oriented gold nanoribbons by the reduction of aqueous chloroaurate ions by hexadecylaniline Langmuir monolayers: Swami, A.; Kumar, A.; Selvakannan, P.R.; Mandal, S.; Pasricha, R.; Sastry, M.	Chemistry of Materials, 2003, 15(1), 17	4.374
Encapsulated HRh(CO)(PPh3)(3) in microporous and mesoporous supports: Novel heterogeneous catalysts for hydroformylation: Mukhopadhyay, K.; Mandale, A.B.; Chaudhari, R.V.	Chemistry of Materials, 2003, 15(9), 1766	4.374
Encapsulated HRh(CO)(PPh3)(3) in microporous and mesoporous supports: Novel heterogeneous catalysts for hydroformylation: Mukhopadhyay, K.; Mandale, A.B.; Chaudhari, R.V.	Chemistry of Materials, 2003, 15(9), 1766	4.374

Title / author	Journal affiliation	IF
Direct assembly of gold nanoparticle "shells" on polyurethanemicrosphere "cores" and their application as Enzyme immobilization templates: Phadtare, S.; Kumar, A.; Vinod, V.P.; Dash, C.; Palaskar, D.V.; Rao, M.; Shukla, P.G.; Sivaram, S.; Sastry, M.	Chemistry of Materials, 2003, 15(10), 1944	4.374
Thermally Evaporated Aerosol OT Thin-Films as Templates for the Room-Temperature Synthesis of Aragonite Crystals: Rautaray, D.; Sainkar, S.R.; Sastry, M.	Chemistry of Materials, 2003, 15(14), 2809	4.049
Self-Assembled Subnanolayers as Interfacial Adhesion Enhancers and Diffusion-Barriers for Integrated-Circuits: Ramanath, G.; Cui, G.; Ganesan, P.G.; Guo, X.; Ellis, A.V.; Stukowski, M.; Vijayamohanan, K.; Doppelt, P.; Lane, M.	Applied Physics Letters , 2003, 83(2), 383	4.049
Influence of various donors on nonlinear I-V characteristics of tin dioxide ceramics: Dhage, S.R.; Ravi, V.	Applied Physics Letters, 2003, 83(22), 4539	4.049
Towards "designer" surfaces: functionalisation of self-assembled monolayer (SAM) on colloidal gold by alkene metathesis: Samanta, D.; Faure, N.; Rondelez, F.; Sarkar, A.	Chemical Communication, 2003, (10), 1186	4.031
Gold nanosheets via reduction of aqueous chloroaurate ions by anthracene anions bound to a liquid-liquid interface: Sanyal, A.; Sastry, M.	Chemical Communication, 2003, (11), 1236	4.031
Barium Hexaaluminate Nanowhiskers Synthesized by Novel Sol-Gel Process in Reverse Micellar Media: Sahu, P.K.; Kulkarni, B.D.; Khomane, R.B.; Pardhy, S.A.; Phalgune, U.D.; Rajmohanan, P.	Chemical Communication, 2003, (15), 1876	4.031
Catalytic ring hydrogenation of phenol under supercritical carbon dioxide: Rode, C.V.; Joshi, U.D.; Sato, O.; Masayuki, S. 4.031	Chemical Communication, 2003 (15), 1960	4.031
Identification of Distinct Bronsted Acidic Sites in Zeolite Mordenite by Proton Localization and (Al-27)-H-1 Reapdor NMR: Ganapathy, S.; Kumar, R.; Delevoye, L.; Amoureux, J.P.	Chemical Communication, 2003, (16), 2076	4.031
Novel CuI/tributyl phosphine catalyst system for amination of aryl chlorides: Patil, N.M.; Kelkar, A.A.; Nabi, Z.; Chaudhari, R.V.	Chemical Communication, 2003, (19), 2460	4.031
Expanding the repertoire of pyrrolidyl PNA analogues for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (Aepone-PNA): Sharma, N.K.; Ganesh, K.N.	Chemical Communication, 2003, (19), 2484	4.031
Two prolines with a difference: contrasting stereoelectronic effects of 4R/S-aminoproline on triplex stability in collagen peptides [Pro(X)-Pro(Y)-Gly](N): Umashankara, M.; Babu, I.R.; Ganesh, K.N.	Chemical Communication, 2003, (20), 2606	4.031

Research papers published (2003)



Biochemical sciences

1. pH-Dependent aggregation of oligomeric Artocarpus hirsuta lectin on thermal denaturation,
Gaikwad, S.M.; Khan, M.I.
Biochem Biophys Res Commun, 2003, **311**(2), 254

2. Detection of genetic variability in pearl millet downy mildew (Sclerospora graminicola) by AFLP,
Singru, R.; Sivaramakrishnan, S.; Thakur, R.P.; Gupta, V.S.; Ranjekar, P.K.
Biochem Genet, 2003, **41**(11-12), 361

3. Equilibrium unfolding of RNase RS from Rhizopus-stolonifer-pHdependeance of chemical and thermal denaturation,
Deshpande, R.A.; Khan, M.I.; Shankar, V.
Biochim Biophys Acta -Proteins and Proteomics, 2003, **1648**(1-2), 184

4. Structural changes enhance the activity of Chainia xylanase in low urea concentrations,
Kumar, A.R.; Hegde, S.S.; Ganesh, K.N.; Khan, M.I.
Biochim Biophys Acta -Proteins Proteomics, 2003, **1645**(2), 164

5. Influence of boron on somatic embryogenesis in papaya,
Renukdas, N.; Mohan, M.L.; Khuspe, S.S.; Rawal, S.K.
Biol Plant, 2003, **47**(1), 129

6. Responses of peanut somatic embryos to thidiazuron,
Joshi, M.V.; Sahasrabudhe, N.A.; Hazra, S.
Biol Plant, 2003, **46**(2), 187

7. Cryopreservation of embryogenic culture of Pinus roxburghii,
Mathur, G.; Alkutkar, V.A.; Nadgauda, R.S.
Biol Plant, 2003, **46**(2), 205

8. Multiple shoot regeneration from immature embryo explants of papaya,
Bhattacharya, J.; Renukadas, N.N.; Khuspe, S.S.; Rawal, S.K.
Biol Plant, 2003, **47**(3), 327

9. Multiple shoot induction and plant regeneration from embryo axes of six cultivars of cotton (Gossypium hirsutum L),
Banerjee, A.K.; Agrawal, D.C.; Nalawade, S.M.; Hazra, S.; Krishnamurthy, K.V.
Biol Plant, 2003, **47**(3), 433

10. Essential polyunsaturated fatty-acid and lipid peroxide levels in never-medicated and medicated schizophrenia patients,
Arvindakhan, M.; Sitasawad, S.; Debsikdar, V.; Ghate, M.; Evans, D.; Horrobin, D.F.; Bennett, C.; Ranjekar, P.K.; Mahadik, S.P.
Biological Psychiatry, 2003, **53**(1), 56

11. Geranium leaf assisted biosynthesis of silver nanoparticles,
Shankar, S.S.; Ahmad, A.; Sastry, M.
Biotechnol Progress, 2003, **19**(6), 1627

12. Candida bombicola cells immobilized on patterned lipid films asenzyme sources for the transformation of arachidonic acid to 20-HETE,
Phadtare, S.; Parekh, P.; Shah, S.; Tambe, A.; Joshi, R.; Sainkar, S.R.; Prabhune, A.; Sastry, M.
Biotechnol Progress, 2003, **19**(6), 1659

13. Optimization of cyclodextrin glycosyltransferase production from klebsiella-pneumoniae as-22 in batch, fed-batch, and continuous cultures,
Gawande, B.N.; Sonawane, A.M.; Jogdand, V.V.; Patkar, A.Y.
Biotechnol Progress, 2003, **19**(6), 1697

14. Aspartic peptidase inhibitors: Implications in drug development,
Dash, C.; Kulkarni, A.; Dunn, B.; Rao, M.
Crit Rev Biochem Molec Biol, 2003, **38**(2), 89

15. Natural history collections: A call for national information infrastructure,
Chavan, V.; Krishnan, S.
Curr Sci, 2003, **84**(1), 34

16. Biosynthesis of metal nanoparticles using fungi and actinomycete,
Sastry, M.; Ahmad, A.; Khan, M.I.; Kumar, R.
Curr Sci, 2003, **85**(2), 162

17. Bud break and plantlet regeneration in vitro from mature trees of Pinus roxburghii Sarg.,
Parasharami, V.A.; Poonawala, I.S.; Nadgauda, R.S.
Curr Sci, 2003, **84**(2), 203

18. Genetic engineering of crop plants for insect resistence,
Ranjekar, P.K.; Patankar, A.; Gupta, V.; Bhatnagar, R.; Bentur, J.; Kumar, P.A.
Curr Sci, 2003, **84**(3), 321

19. Electronic catalogue of known Indian fauna,
Chavan, V.; Watve, A.; Krishnan, S.
Curr Sci, 2003, **85**(11), 1515

20. Genetic diversitat in Vitiaestivati Nachkommen,
Agarwal, D.C.; Eibach, Rudalf; Zyprian, Eva
Deulsches Weinbau-Jahrbuch, 2003, **54**, 79

21. Biosynthesis of cholesterol oxidase by streptomyces-lavendulae NCIM-2421,
Varma, R.; Nene, S.
Enzyme Microb Technol, 2003, **33**(2-3), 286

22. Biodeinking of mixed office waste paper by alkaline active cellulases from alkalotolerant Fusarium sp.,
Vyas, S.; Lachke, A.
Enzyme Microb Technol, 2003, **32**(2), 236

23. Purification, characterization and mode of action of an endo-polygalacturonase from the psychrophilic fungus mucor flavus,
Gadre, R.V.; Gonzalez, V.D.; Josef, V.B.; Bhat, M.K.
Enzyme Microb Technol, 2003, **32**, 321

24. Genetic relationships among annual and perennial wild species of Cicer using inter simple sequence repeat (ISSR) polymorphism,
Rajesh, P.N.; Sant, V.J.; Gupta, V.S.; Muehlbauer, F.J.; Ranjekar, P.K.
Euphytica, 2003, **129**(1), 15

25. Single-strand-specific nucleases,
Desai, N.A.; Shankar, V.
Fems Microbiol Rev, 2003, **26**(5), 457

26. Fabrication of a laboratory scale flotation cell device for bio-deinking of waste papers,
Vyas, S.; Sainkar, S.R.; Lachke, A.
Indian J Chem Technology, 2003, **10**(6), 593

27. Influence of plant allelochemicals on growth-rate, nutritional physiology and midgut esterase-activity in 5th instar larvae of spodoptera-litura (f) (lepidoptera-noctuidae),
Mukherjee, S.
Inverteb Reprod Development, 2003, **43**(2), 125

28. Effect of sublethal concentrations of flufenoxuron on growth, development and reproductive-performance of tribolium-castaneum (Herbst) (Coleoptera-tenebrionidae),
Salokhe, S.G.; Pal, J.K.; Mukherjee, S.N.
Inverteb Reprod Development, 2003, **43**(2), 141

29. Stability of β-carotene in spray-dried preparation of rhodotorula-glutinis mutant-32,
Bhosale, P.; Jogdand, V.V.; Gadre, R.V.
J Appl Microbiol, 2003, **95**(3), 584

30. Slow tight binding inhibition of proteinase K by a proteinaceous inhibitor -conformational alterations responsible for conferring irreversibility to the enzyme-inhibitor complex,
Pandhare, J.; Dash, C.; Rao, M.; Deshpande, V.
J Biol Chem, 2003, **278**(49), 48735

31. Tailor made functional surfaces: Potential elastomeric biomaterials I,
Desai, S.M.; Bodas, D.; Patil, K.R.; Patole, M.; Singh, R.P.
J Biomat Sci : Polym Ed, 2003, **14**, 1323

32. Bioprospecting the lat gene in soil samples,
Dharwadkar, A.; Gupta, V.; Pant, A.
J Biosciences, 2003, **28**(5), 597

33. Poly(3-hydroxybutyrate) (PHB) synthesis by recombinant Escherichia coli harbouring Streptomyces aureofaciens PHB biosynthesis genes: Effect of various carbon and nitrogen sources,
Mahishi, L.H.; Tripathi, G.; Rawal, S.K.
Microbiol Res, 2003, **158**(1), 19

34. Identification of potent inhibitors of helicoverpa-armigera gut proteinases from winged bean-seeds,
Giri, A.P.; Harsulkar, A.M.; Ku, M.S.B.; Gupta, V.S.; Deshpande, V.V.; Ranjekar, P.K.; Franceschi, V.R.
Phytochemistry, 2003, **63**(5), 523

35. Bitter gourd proteinase-Inhibitors -potential growth-Inhibitors of helicoverpa-armigera and spodoptera-litura,
Telang, M.; Srinivasan, A.; Patankar, A.; Harsulkar, A.; Joshi, V.; Damle, A.; Deshpande, V.; Sainani, M.; Ranjekar, P.
Phytochemistry, 2003, **63**(6), 643

36. Differential inhibition of helicoverpa-armigera gut proteinases by proteinase-inhibitors of pigeonpea (cajanus-cajan) and its wild relatives,
Chougule, N.P.; Hivrale, V.K.; Chhabda, P.J.; Giri, A.P.; Kachole, M.S.
Phytochemistry, 2003, **64**(3), 681

37. Molecular marker analysis of kernel size and shape in bread wheat,
Dholakia, B.B.; Ammiraju, J.S.; Singh, H.; Lagu, M.D.; Roder, M.S.; Rao, V.S.; Dhaliwal, H.S.; Ranjekar, P.K.; Gupta, V.S.
Plant Breed, 2003, **122**(5), 392

38. Influence of medium composition on callus induction and camptothecin(S) accumulation in Nothapodytes foetida,
Thengane, S.R.; Kulkarni, D.K.; Shrikhande, V.A.; Joshi, S.P.; Sonawane, K.B.; Krishnamurthy, K.V.
Plant Cell Tissue Organ Cult, 2003, **72**(3), 247

39. Supplementation with a combination of ω-3-fatty-acids and antioxidants (vitamins-e and vitamins-c) improves the outcome of schizophrenia,
Arvindakshan, M.; Ghate, M.; Ranjekar, P.K.; Evans, D.R.; Mahadik, S.P.
Schizophr Res, 2003, **62**(3), 195

40. Direct induction of somatic embryogenesis from immature zygotic embryo of cashewnut (Anacardium occidentale L.),
Gogate, S.S.; Nadgauda, R.S.
Sci Hort Amsterdam, 2003, **97**(1), 75

41. Direct induction of somatic embryogenesis from immature zygotic embryo of cashewnut (Anacardium occidentale L.),
Gogate, S.S.; Nadgauda, R.S.
Scientia Horticulturae, 2003, **97**(1), 75

42. Terpenoid metabolism in wild-type and transgenic arabidopsis plants,
Aharoni, A.; Giri, A.P.; Deuerlein, S.; Griepink, F.; Kogel, W.; Verstappen, F.W.A.; Verhoeven, H.A.; Jongsma, M.A.; Schwab, W.; Bouwmeester, H.J.
The Plant cell, 2003, **15**(12), 2866

43. Influence of pre-bloom sprays of benzyladenine on in vitro recovery of hybrid embryos from crosses of thompson seedless and 8 seeded varieties of grape (Vitis spp),
Bharathy, P.V.; Karibasappa, G.S.; Biradar, A.B.; Kulkarni, D.D.; Solanke, A.U.; Patil, S.G.; Agrawal, D.C.
Vitis, 2003, **42**(4), 199

Catalysis

1. Effect of nonframework cations and crystallinity on the Basicityof Nax Zeolites,
Joshi, U.D.;Joshi, P.N.;Tamhankar, S.S.;Joshi, V.V.;Rode, C.V.;Shiralkar, V.P.
Appl Catal A Gen, 2003, **239**(1-2), 209

2. Preparation of isobutylcumenes by liquid-phase isopropylation of isobutylbenzene with 2-propanol using zeolite H-β,
Venkatesan, C.; Chidambaram, M.; Kamble, K.R.; Singh, A.P.
Catal Lett, 2003, **85**(3-4), 171

3. New aliphatic C-Metalated palladacycle in the pores of 3-Hydroxypropyl triethoxysilane functionalized Mcm-41,
Venkatsan, C.; Singh, A.P.
Catal Lett, 2003, **88**(3-4), 193

4. Epoxidation of styrene by anhydrous H_2O_2 over TS-1 and Gamma-Al_2O_3 catalysts -effect of reaction water, poisoning of acid sites and presence of base in the reaction mixture ,
Choudhary, V.R.; Patil, N.S.; Bhargava, S.K.
Catal Lett, 2003, **89**(1-2), 55

5. Synthesis of cyclic carbonates from olefins and CO_2 over zeolite-based catalysts,
Srivastava, R.; Srinivas, D.; Ratnasamy, P.
Catal Lett, 2003, **89**(1-2), 81

6. Synthesis of polycarbonate precursors over titanosilicate molecular sieves,
Srivastava, R.; Srinivas, D.; Ratnasamy, P.
Catal Lett, 2003, **91**(1-2), 133

7. Oxidative dehydrogenation of ethylbenzene over Cu1-xCoxFe$_2$O$_4$ catalyst system: influence of acid-base property,
Mathew, T.; Malwadkar, S.; Shivanand, d.; Pai, i.; Sharanappa, N.; Sebastian, C.P.; Satyanarayana, C.V.; Bokade, V.V.
Catal Lett, 2003, **91**(3-4), 217

8. Biomimetic oxidations using transition metal complexes encapsulated in zeolites,
Srinivas, D.; Sivasanker, S.
Catal Surv Asia, 2003, **7**(2-3), 121

9. Experimental and computational study of liquid drop over flat and spherical surfaces,
Gunjal, P.R.; Ranade, V.V.; Chaudhari, R.V.
Catal Today, 2003, **79**(1-4), 267

10. Activity and selectivity of Rh-complex catalysts in hydroformylation of 1,4-diacetoxy-butene to vitamin A intermediate,
Chansarkar, R.; Mukhopadhyay, K.; Kelkar, A.A.; Chaudhari, R.V.
Catal Today, 2003, **79**(1-4), 51

11. Decomposition of NO and N_2O on Cu-Alts-1 -oscillatory behavior at full N_2O conversion,
Schay, Z.; Guczi, L.; Palborbely, G.; Ramaswamy, A.V.
Catal Today, 2003, **84**(3-4), 165

12. Kinetics of hydrogenation of maleic-acid in a batch slurry reactor using a bimetallic Ru-Re/C catalyst,
Chaudhari, R.V.; Rode, C.V.; Deshpande, R.M.; Jaganathan, R.; Leib, T.M.; Mills, P.L.
Chem Engg Sci, 2003, **58**(3-6), 627

13. Reactive oxygen species in epoxidation reactions over titanosilicate molecular sieves,
Shetti, V.N.; Manikandan, P.; Srinivas, D.; Ratnasamy, P.
J Catal, 2003, **216**(1-2), 461

14. Alkylation of o-toluidine with methanol over acidic zeolites,
Anand, R.; Maheswari, R.; Hegde, S.G.; Rao, B.S.
J Mol Catal A -Chem, 2003, **192**(1-2), 253

15. Tertiary butylation of phenol over HY and dealuminated HY zeolites,
Anand, R.; Maheswari, R.; Gore, K.U.; Tope, B.B.
J Mol Catal A -Chem, 2003, **193**(1-2), 251

16. Reaction kinetics of the selective liquid phase hydrogenation of styrene oxide to β-phenethyl alcohol,
Rode, C.V.; Telkar, M.M.; Jaganathan, R.; Chaudhari, R.V.
J Mol Catal A -Chem, 2003, **200**(1-2), 279

17. Al-MCM-41 catalyzed alkylation of phenol with methanol,
Bhattacharya, K.G.; Talukdar, A.K.; Das, P.; Sivasanker, S.
J Mol Catal A-Chem, 2003, **197**(1-2), 255

18. Aniline as a stabilizer for metal nanoparticles,
Athawale, A.A.; Bhagwat, S.V.; Katre, P.P.; Chandwadkar, A.J.; Karandikar, P.
Mater Lett, 2003, **57**(24-25), 3889

19. Synthesis of nanocrystalline SnO_2 powder by amorphous citrate route,
Bhagwat, M.; Shah, P.; Ramaswamy, V.
Mater Lett, 2003, **57**(9-10), 1604

20. Multinuclear (Al-27, Si-29, Ti-47,Ti-49) solid-state NMR of titanium substituted zeolite USY,
Ganapathy, S.; Gore, K.U.; Kumar, R.; Amoureux, J.P.
Solid State Nuclear Magn Resonance, 2003, **24**(2-3), 184

21. O-methylation of dihydroxybenzenes with methanol in the vapour phase over alkali-loaded SiO_2 catalysts: A kinetic analysis,
Bal, R.; Mayadevi, S.; Sivasanker, S.
Org Process Res Dev, 2003, **7**(1), 17

22. Synthesis and structural characterization of AlPO4-18 and magnesium and zinc substituted AlPO4-18,
Bhagwat, M.; Satyanarayana, C.V.V; Ramaswamy, V.
Bull Catal Soc India, 2003, **2**, 60

23. Friedel-Crafts type benzylation and benzoylation of aromatic compounds over H β zeolite modified by oxides or chlorides of gallium and indium,
Choudhary, V.R.; Jana, S.K.; Patil, N.S.; Bhargava, S.K.
Microporous Mesoporous Mat, 2003, **57**(1), 21

24. Catalysis research in India and the role of the catalysis society of India.
Ramaswamy, A.V.; Sivasanker, S.
Catal Surv Asia, 2003, **7**(1), 91

25. Kinetics of hydrogen peroxide decomposition in aqueous sulfuric acid over palladium/carbon: Effect of acid concentration,
Choudhary, V.R.; Gaikwad, A.G.
React Kinet Catal Lett, 2003, **80**(1), 27

26. Solvent-free liquid phase oxidation of benzyl alcohol to benzaldehyde by molecular oxygen using non-noble transition metal containing hydrotalcite-like solid catalysts,
Choudhary, V.R.; Chaudhari, P.A.; Narkhede, V.S.
Catal Commun, 2003, **4**(4), 171

27. Synthesis of p-aminophenol by catalytic hydrogenation of p-nitrophenol,
Vaidya, M.J.; Kulkarni, S.M.; Chaudhari, R.V.
Org Process Res Dev, 2003, **7**(2), 202

28. Hydrogenation of olefins over hydrido chlorocarbonyl tris-(triphenylphosphine) ruthenium (II) complex immobilized on functionalized MCM-41 and SBA-15,
Joseph, T.; Vinu, A.; Deshpande, S.S.; Hartmann, M.; Ernst, S.; Halligudi, S.B.
J Mol Catal A -Chem, 2003, **206**, 13

29. Design of solid base catalysts for the production of chemicals,
Sivasanker, S.
Stud Surf Sci Catal, 2003, **145**, 85

30. Preparation and stabilization of gold nanoparticles formed by in-situ reduction of aqueous chloroaurate ions within surface-modified mesoporous silica,
Ghosh, A.; Patra, C.R.; Mukherjee, P.; Sastry, M.; Kumar, R.
Microporous and Mesoporous Mat, 2003, **58**(3), 201

31. Synthesis of acid functionalized mesoporous Zr-O-SO2-CF3 catalysts; heterogenization of CF3SO3H over mesoporous Zr(OH)(4),
Chidambaram, M.;Venkatesan, C.;Rajamohanan, P.R.;Singh, A.P.
Appl Catal A Gen, 2003, **244**(1), 27

32. Heterogenized HRh(CO)(PPh3)(3) on zeolite Y using phosphotungstic acid as tethering agent: a novel hydroformylation catalyst,
Mukhopadhyay, K.; Chaudhari, R.V.
J Catal, 2003, **213**(1), 73

33. An improved process for the synthesis of VPI-5 molecular sieve,
Venkatathri, N.
Bull Mater Sci, 2003, **26**(3), 279

34. Solvent free selective oxidation of benzyl alcohol and benzaldehyde by tert-butyl hydroperoxide using MnO4 exchanged Mg-Al-hydrotalcite catalysts,
Choudhary, V.R.; Dumbre, D.K.; Markhede, V.S.; Jana, S.K.
Catal Lett, 2003, **86**(4), 229

35. Combustion of dilute propane over transition metal-doped ZrO2 (Cubic) catalysts,
Choudhary, V.R.;Banerjee, S.;Pataskar, S.G.
Appl Catal A Gen, 2003, **253**(1), 65

36. Oxidation of Adamantane by urea hydroperoxide using vanadium complex anchored onto functionalized Si-MCM-41,
Joseph, T.; Hartmann, M.; Halligudi, S.B.; Ernst, S.
J Mol Catal A -Chem, 2003, **207**(2), 131

37. Alkali promoted selective epoxidation of styrene to styrene oxide using TS-1 catalyst,
Rode, C.V.; Nehete, U.N.; Dongare, M.K.
Catal Commun, 2003, **4**, 365

38. Aromatization of n-heptane over H-AlMFI, Ga/H-AlMFI, H-GaMFI and H-GaAlMFI zeolite catalysts: influence of zeolitic acidity and non-framework gallium,
Choudhary, V.R.; Mulla, S.A.; Banerjee, S.
Microporous Mesoporous Mat, 2003, **57**(3), 317

39. Reactive oxo-titanium species in titanosilicate molecular sieves EPR investigations and structure activity correlations,
Srinivas, D.; Manikandan, P.; Laha, S.C.; Kumar, R.; Ratnasamy, P.
J Catal, 2003, **217**(1), 160

40. Temperature-programmed desorption of water and ammonia on sulfated zirconia catalysts for measuring their strong acidity and acidity distribution,
Choudhary, V.R.; Karkamkar, A.J.
Proc Indian Acad Sci-Chem, 2003, **115**(4), 281

41. Synthesis of nanocrystalline titania using ultrasonication technique and its photocatalytic activity for the decomposition of monochlorobenzene,
Awati, P.; Awate, S.; Shah, P.; Ramaswamy, V.
Catal Commun, 2003, **4**, 393

42. Low-temperature complete combustion of dilute propane over mn-doped ZrO2 (cubic) catalysts,
Choudhary, V.R.; Banerjee, S.; Pataskar, S.G.
Proc Indian Acad Sci-Chem, 2003, **115**(4), 287

43. N-alkylation of aniline with ethanol over HY and dealuminated HY zeolites,
Anand, R.;Khaire, S.S.;Maheswari, R.;Gore, K.U.;Chumbhale, V.R.
Appl Catal A Gen, 2003, **242**(1), 171

44. Microwave assisted solvent-free synthesis of dihydropyrimidinones by Biginelli reaction over Si-MCM- 41 supported FeCl3 catalyst,
Choudhary, V.R.; Tillu, V.H.; Narkhede, V.S.; Borate, H.B.; Wakharkar, R.D.
Catal Commun, 2003, **4**(9), 449

45. Mixing in bubble columns reactors: Role of unsteady flow structures,
Buwa, V.V.; Ranade, V.V.
Canadian J Chem Engg, 2003, **81**, 402

46. Isopropylation of naphthalene over modified faujasites: effect of steaming temperature on activity and selectivity,
Anand, R.;Maheswari, R.;Gore, K.U.;Khaire, S.S.;Chumbhale, V.R.
Appl Catal A Gen, 2003, **249**(2), 265

47. Titanium silicates for carbon-carbon bond formation reactions,
Sasidharan, M.; Kumar, R.
J Catal, 2003, **220**(2), 326

48. Reaction kinetics studies on catalytic dehydration of 1,4-butanediol using cation exchange resin,
Vaidya, S.H.;Bhandari, V.M.;Chaudhari, R.V.
Appl Catal A Gen, 2003, **242**(2), 321

49. Structural studies on NiO-CeO2-ZrO2 catalysts for steam reforming of ethanol,
Srinivas, D.;Satyanarayana, C.V.V;Potdar, H.S.; Ratnasamy, P.
Appl Catal A Gen, 2003, **246**(2), 323

50. Vapor-phase selective O-alkylation of phenol over alkali loaded silica,
Bal, R.;Sivasanker, S.
Appl Catal A Gen, 2003, **246**(2), 373

51. Conversion of ethane to ethylene in presence of limited O-2 over supported SrO promoted SM2O3 catalyst,
Mulla, S.A.R.; Choudhary, V.R.
Indian J Chem Technology, 2003, **10**(6), 615

52. Synthesis and characterization of vanadium containing ATO-and AFO-type molecular sieves,
Venkatathri, N.
Appl Catal A Gen, 2003, **242**(2), 393

53. Synthesis and characterization of triflic acid-functionalized mesoporous Zr-TMS catalysts: heterogenization of CF3SO3H over Zr-TMS and its catalytic activity,
Chidambaram, M.; CurullaFerre, D.; Singh, A.P.; Anderson, B.G.
J Catal, 2003, **220**(2), 442

54. An and Au-Pt bimetallic nanoparticles in MCM-41 materials -applications in Co preferential oxidation,
Chilukuri, S.; Joseph, T.; Malwadkar, S.; Damle, C.; Halligudi, S.B.; Rao, B.S.; Sastry, M.; Ratnasamy, P.
Stud Surf Sci Catal, 2003, **146**, 573

55. Modelling of gas-liquid / gas-liquid-solid flows in bubble column reactors,
Rampure, M.R.; Buwa, V.V.; Ranade, V.V.
Canadian J Chem Engg, 2003, **81**(3), 692

56. Liquid distribution and RTD in trickle bed reactor: Experiments and CFD simulations,
Gunjal, P.R.; Ranade, V.V.; Chaudhari, R.V.
Canadian J Chem Engg, 2003, **81**(3), 821

57. Studies on Vanadium incorporation in AFI type molecular-sieves,
Venkatathri, N.; Hegde, S.G.; Sivasanker, S.
Indian J Chem A, 2003, **42**(5), 974

58. Saturated N-heterocyclic carbene oxime and amine palladacycle catalysis of the Mizoroki-Heck and the Suzuki reactions,
Iyer, S.; Jayanthi, A.
Synlett, 2003, (8), 1125

59. Rietveld refinement study of nanocrystalline copper doped zirconia,
Bhagwat, M.; Ramaswamy, A.V.; Tyagi, A.K.; Ramaswamy, V.
Mater Res Bull, 2003, **38**(13), 1713

60. Encapsulated HRh(CO)(PPh3)(3) in microporous and mesoporous supports: novel heterogeneous catalysts for hydroformylation,
Mukhopadhyay, K.; Mandale, A.B.; Chaudhari, R.V.
Chem Mater, 2003, **15**(9), 1766

61. Barium hexaaluminate nanowhiskers synthesized by novel sol-gel process in reverse micellar media,
Sahu, P.K.; Kulkarni, B.D.; Khomane, R.B.; Pardhy, S.A.; Phalgune, U.D.; Rajmohanan, P.
Chem Commun, 2003, (15), 1876

62. Catalytic ring hydrogenation of phenol under supercritical carbon dioxide,
Rode, C.V.; Joshi, U.D.; Sato, O.; Masayuki, S.
Chem Commun, 2003, 1960

63. Heck reaction over Pd-loaded ETS-10 molecular-sieve,
Waghmode, S.B.; Wagholikar, S.G.; Sivasanker, S.
Bull Chem Soc Japan, 2003, **76**(10), 1989

64. Identification of distinct bronsted acidic sites in zeolite mordenite by proton localization and (Al-27)-H-1 reapdor NMR,
Ganapathy, S.; Kumar, R.; Delevoye, L.; Amoureux, J.P.
Chem Commun, 2003, (16), 2076

65. Ruthenium-catalyzed ring-closing metathesis on alkene-tethered fischer carbene complexes,
Hazra, D; Sarkar, A.
Indian J Chem A, 2003, **42**(9), 2398

66. Novel CuI/tributyl phosphine catalyst system for amination of aryl chlorides,
Patil, N.M.; Kelkar, A.A.; Nabi, Z.; Chaudhari, R.V.
Chem Commun, 2003, (19), 2460

67. Kinetic modeling of carbonylation of 1-(4-Isobutylphenyl) ethanolusing a homogeneous PdCl2 (pph3)(2)/ Tsoh/LiCl catalyst system,
Seayad, A.M.; Seayad, J.; Mills, P.L.; Chaudhari, R.V.
Ind Engg Chem Res, 2003, **42**(12), 2496

68. Eulerian flow-field estimation from particle trajectories numerical experiments for stirred tank type flows,
Rammohan, A.R.; Dudukovic, M.P.; Ranade, V.V.
Ind Engg Chem Res, 2003, **42**(12), 2589

69. Synthesis and characterization of AlPO4-5 from aqueous and non-aqueous systems using hexamethyleneimine template,
Venkatathri, N.
Indian J Chem A, 2003, **42**(11), 2717

70. Facile and selective deprotection of allyl esters catalyzed by H-β zeolite,
Pandey, R.K.; Kadam, V.S.; Upadhyay, R.K.; Dongare, M.K.; Kumar, P.
Synthetic Commun, 2003, **33**(17), 3017

71. Modeling of hydrogenation of maleic acid in a bubble-column slurry reactor,
Thakar, N.N.;Jaganathan, R.;Chaudhari, R.V.;Mills, P.L.
Aiche J, 2003, **49**(12), 3199

72. Pd-SAPO-31, an efficient, heterogeneous catalyst for Heck reactions of aryl chlorides,
Srivastava, R.; Venkatathri, N.; Srinivas, D.; Ratnasamy, P.
Tetrahedron Lett, 2003, **44**(18), 3649

73. Synthesis of carbamates using yttria-zirconia based Lewis acid catalyst,
Pandey, R.K.; Dagade, S.P.; Dongare, M.K.; Kumar, P.
Synthetic Commun, 2003, **33**(23), 4019

74. Eco-benign mesoporous materials for organic-reactions
Raja, T.; Horniakova, J.; Jacob, N.E.; Jha, R.K.; Kubota, Y.; Sugi, Y,
Mater Sci Forum, 2003, **426**, 4623

75. Physicochemical investigations of the basicity of the cation-exchanged ETS-10 molecular-sieves,
Waghmode, S.B.; Vetrivel, R.; Hegde, S.G.; Gopinath, C.S.; Sivasanker, S.
J Phys Chem B, 2003, **107**(33), 8517

Engineering sciences

1. Kinetic modeling of liquid phase oxidation of cyclohexane,
Bhattacharya, A.; Mungikar, A.
Canadian J Chem Engg, 2003, **81**(2), 220

2. Simulation of flows in stirred vessels agitated by dual rushtonimpellers using computational snapshot approach,
Deshpande, V.R.; Ranade, V.V.
Chem Engg Comm, 2003, **190**(2), 236

3. Support vector machines -A useful tool for process engineering applications,
Agarwal, M.; Jade, A.M.; Jayaraman, V.K.; Kulkarni, B.D.
Chem Engg Prog, 2003, **99**(1), 57

4. Thermodynamic study of reaction of phenol with methanol over Cu1-xCoxFe2O4 (X=0, 0.25, 0.50, 0.75 and 1) spinel system,
Mathew, T.; Shiju, N.R.; Nimje, R.Y.; Adkine, P.M.; Rao, B.S.; Bokade, V.V.
Chem Engg Res Des, 2003, **81**(A2), 265

5. Feature extraction and denoising using kernel PCA,
Jade, A.M.; Srikanth, B.; Jayaraman, V.K.; Kulkarni, B.D.; Jog, J.P.; Priya, L.
Chem Engg Sci, 2003, **58**(19), 4441

6. Computational fluid dynamics(CFD) for design, scale-up and process intensification,
Utikar, R.P.; Ranade, V.V.
Chem Ind Digest, 2003, **XVI**, 42

7. Artificial neural networks for prediction of mycobacterial promoter sequences,
Kalate, R.N.; Tambe, S.S.; Kulkarni, B.D.
Comput Biol Chem, 2003, **27**(6), 555

8. Bubbling columns,
Buwa, V.V.; Ranade, V.V.
Fluent Newsletter, 2003, **XII**, 10

9. Computational Fluid dynamics for designing process equipment -expectations, current status and path forward,
Joshi, J.B.; Ranade, V.V.
Ind Engg Chem Res, 2003, **42**(6), 1115

10. Gas-liquid flow generated by a pitched-blade turbine: particle image velocimetry measurements and computational fluid dynamics simulations,
Khopkar, A.R.; Aubin, J.; Xuereb, C.; LeSauze, N.; Bertrand, J.; Ranade, V.V.
Ind Engg Chem Res, 2003, **42**(21), 5318

11. Memory based local learning: application to processing engineering problems,
Kulakrni, A.; Patil, S.V.; Jayaraman, V.K.; Kulkarni, B.D.
Int J Chem React Engg, 2003, **1A**, 23

12. Studies in effective utilization of biomass chemical modification of bagasse and mechanism of color removal,
Mane, J.D.; Kumbhar, D.L.; Barge, S.C.; Phadnis, S.P.; Bhandari, V.M.
Int Sugar J, 2003, **105**(1257), 412

13. Role of heat-transfer and thermal-conductivity in the crystallization behavior of polypropylene-containing additives -a phenomenological model,
Radhakrishnan, S.; Sonawane, P.S.
J Appl Polym Sci, 2003, **89**(11), 2994

14. Liquid-liquid equilibria for the epichlorohydrin plus water plus methanol and allyl chloride plus water plus methanol systems,
Vaidya, P.S.; Naik, R.V.
J Chem Engg Data, 2003, **48**(4), 1015

15. Some studies on energy savings in sponge iron plants,
Biswas, D.K.; Asthana, S.R.; Rau, V.G.
J Ener Resour Techno Trans Am Soc Mech engr (ASME, 2003, **125**, 228

16. Statistical analysis of the physicochemical data on the coastal waters of Cochin,
Iyer, C.S.P.; Sindhu, M.; Kulkarni, S.G.; Tambe, S.S.; Kulkarni, B.D.
J Environmental Monitoring, 2003, **5**(2), 324

17. A tabu search based approach for solving a class of bilevel programming problems in chemical engineering,
J, R.; Gupta, K.; Kusumakar, H.S.; Jayaraman, V.K.; Kulkarni, B.D.
J Heuristics, 2003, **9**(4), 307

18. Solid state electrochemical reactions in photocells made using conducting polyaniline and sensitized with methylene blue,
Somani, P.; Radhakrishnan, S.
J Solid State Electrochem, 2003, **7**, 166

19. Shear induced demixing and rheological behaviour of aqueous solutions of poly(N-Isopropylacrylamide),
Badiger, M.V.; Wolf, B.A.
Macromol Chem Phys, 2003, **204**(4), 600

20. Multiobjective optimization of reactor-regenerator system using ant algorithm,
Shelokar, P.S.; Jayaraman, V.K.; Kulkarni, B.D.
Petroleum Sci Technol, 2003, **21**(7-8), 1167

21. Control of chaotic dynamical systems using support vector machines,
Kulkarni, A.; Jayaraman, V.K.; Kulkarni, B.D.
Phys Lett A, 2003, **317**(5-6), 429

Materials sciences

1. Room-temperature synthesis of aragonite crystals at an expanding liquid-liquid interface in a radial Hele-Shaw cell,
Rautaray, D.;Banpurkar, A.;Sainkar, S.R.;Limaye, A.V.;Pavaskar, N.R.;Ogale, S.B.;Sastry, M.
Advan Mater, 2003, **15**(15), 1273

2. Self-assembled subnanolayers as interfacial adhesion enhancers and diffusion-barriers for integrated-circuits,
Ramanath, G.;Cui, G.;Ganesan, P.G.;Guo, X.;Ellis, A.V.;Stukowski, M.;Vijayamohanan, K.;Doppelt, P.;Lane,M.
Appl Phys Lett, 2003, **83**(2), 383

3. Influence of various donors on nonlinear I-V characteristics oftin dioxide ceramics,
Dhage, S.R.; Ravi, V.
Appl Phys Lett, 2003, **83**(22), 4539

4. Preparation of microwave dielectric, Sn0.2Zr0.8TiO4,
Dhage, S.R.; Ravi, V.; Date, S.K.
Bull Mater Sci, 2003, **26**(2), 215

5. On the morphology of SrCO3 crystals grown at the interface between two immiscible liquids,
Reddy, S.; Rautaray, D.; Sainkar, S.R.; Sastry, M.
Bull Mater Sci, 2003, **26**(3), 283

6. Gold nanosheets via reduction of aqueous chloroaurate ions by anthracene anions bound to a liquid-liquid interface,
Sanyal, A.; Sastry, M.
Chem Commun, 2003, (11), 1236

7. Highly oriented gold nanoribbons by the reduction of aqueous chloroaurate ions by hexadecylaniline,
Langmuir monolayers. Swami, A.; Kumar, A.; Selvakannan, P.R.; Mandal, S.; Pasricha, R.; Sastry, M.
Chem Mater, 2003, **15**(1), 17

8. Direct assembly of gold nanoparticle "shells" on polyurethanemicrosphere "cores" and their application as enzyme immobilization templates,
Phadtare, S.; Kumar, A.; Vinod, V.P.; Dash, C.; Palaskar, D.V.; Rao, M.; Shukla, P.G.; Sivaram, S.; Sastry, M.
Chem Mater, 2003, **15**(10), 1944

9. Thermally evaporated aerosol ot thin-films as templates for the room-temperature synthesis of aragonite crystals,
Rautaray, D.; Sainkar, S.R.; Sastry, M.
Chem Mater, 2003, **15**(14), 2809

10. Enhanced supercapacitance of multiwalled carbon nanotubes functionalized with ruthenium oxide,
Arabale, G.; Wagh, D.; Kulkarni, M.; Mulla, I.S.; Vernekar, S.P.; Vijayamohanan, K.; Rao, A.M.
Chem Phys Lett, 2003, **376**(1-2), 207

11. Energies and dipole moments of excited states of ozone and ozone radical cation using Fock space multireference coupled-cluster analytical response approach,
Devarajan, A.; Hirao, K.; Pal, S.
Collect Czech Chem Commun, 2003, **68**(1), 47

12. Protein diffusion into thermally evaporated lipid films: role of protein charge/mass ratio,
Gole, A.; Thakar, J.; Sastry, M.
Colloid Surface B, 2003, **28**(2-3), 209

13. Extracellular biosynthesis of silver nanoparticles using the fungus Fusarium oxysporum,
Ahmad, A.; Mukherjee, P.; Senapati, S.; Mandal, D.; Khan, M.I.; Kumar, R.; Sastry, M.
Colloid Surface B, 2003, **28**(4), 313

14. Highly organized assembly of BaSO4 crystals grown within thermally evaporated AOT thin films,
Rautaray, D.; Sainkar, S.R.; Sastry, M.
Cryst Eng Comm, 2003, **5**, 400

15. BaSO4 crystals grown at an expanding liquid-liquid interface in a radial Hele-Shaw Cell show spontaneous large-scale assembly into filaments,
Rautaray, D.; Banpurkar, A.; Sainkar, S.R.; Limaye, A.V.; Ogale, S.; Sastry, M.
Cryst Growth Des, 2003, **3**(4), 449

16. Device applications of self-assembled monolayers and monolayer-protected nanoclusters,
Aslam, M.; Chaki, N.K.; Sharma, J.; Vijayamohanan, K.
Curr Appl Phys, 2003, **3**(2-3), 115

17. Assembling gold nanoparticles in solution using phosphorothioate DNA as structural interconnects,
Kumar, A.; Phadtare, S.; Pasricha, R.; Guga, P.; Ganesh, K.N.; Sastry, M.
Curr Sci, 2003, **84**(1), 71

18. Phase transfer protocols in nanoparticle synthesis,
Sastry, M.
Curr Sci, 2003, **85**, 1735

19. Varistors based on doped SnO2,
Dhage, S.R.; Samuel, V.; Ravi, V.
Electroceramics, 2003, **11**(1-2), 81

20. A Novel magnetic exchange mechanism in bridged copper (II)coordinations of naturally occuring spin carriers viz. orthofunctionalized P-napthoquinones,
Rane, S.; Gawali, S.; Padhye, S.; Date, S.K.; Bakare, P.P.
Indian J Chem A, 2003, **42**(2), 255

21. Metal-ion complexes of the optically pure Bi(4-phenyl-1, 3-oxazoline) ligand -synthesis, characterization and X-ray crystal structures,
Patra, G.K.; Goldberg, I.; Sarkar, A.; Chowdhury, S.; Datta, D.
Inorg Chim Acta, 2003, **344**(Feb), 7

22. Keggin Ions as UV-switchable reducing agents in the synthesis of Au core-Ag shell nanoparticles,
Mandal, S.; Selvakannan, P.R.; Pasricha, R.; Sastry, M.
J Am Chem Soc, 2003, **125**(28), 8440

23. Biosynthesis of CaCO3 crystals of complex morphology using a fungus and an actinomycete,
Rautaray, D.; Ahmad, A.; Sastry, M.
J Am Chem Soc, 2003, **125**(48), 14656

24. Effect of chain-length on the tunneling conductance of gold quantum dots at room-Temperature,
Chaki, N.K.; Gopakumar, T.G.;
Maddanimath, T.; Aslam, M.; Vijayamohanan, K.
J Appl Phys, 2003, **94**(5), 3663

25. Effect of carbon black on the mechanical and dielectric properties of rubber ferrite composites containing barium ferrite,
Soloman, M.A.; Kurian, P.; Anantharaman, M.R.; Joy, P.A.
J Appl Polym Sci, 2003, **89**(3), 769

26. Speed of sound in concentrated aqueous KCl solutions from 278.15 to 338.15 K,
Kumar, A.
J Chem Engg Data, 2003, **48**(2), 388

27. Effect of temperature on the volumetric properties of the L-alanine (1) + KCl (2) + H2O (3) system,
Badarayani, R.; Kumar, A.
J Chem Engg Data, 2003, **48**(3), 664

28. A study of electronic and bonding properties of Sn doped Li-n clusters and aluminum based binary clusters through electron localization function,
Shetty, S.; Pal, S.; Kanhere, D.G.
J Chem Phys, 2003, **118**(16), 7288

29. Enhancement of photoluminescence in manganese doped ZnS nanoparticles due to a silica shell,
Ethiraj, A.S.; Hebalkar, N.; Kulkarni, S.K.; Pasricha, R.; Urban, J.; Dem, C.; Schmitt, M.; Kiefer, W.; Weinhardt, L.; Joshi, S.
J Chem Phys, 2003, **118**(19), 8945

30. Density functional response approach for the linear and nonlinear electric properties of molecules,
Sophy, K.B.; Pal, S.
J Chem Phys, 2003, **118**(24), 10861

31. Densities and speed of sound of glycine on concentrated aqueous NaBr, KCl, KBr and MgCl(2) at T=298.15 K,
Badarayani, R.; Kumar, A.
J Chem Thermodynamics, 2003, **35**(6), 897

32. Langmuir-Blodgett films of laurylamine-modified hydrophobic gold nanoparticles organized at the air-water interface,
Swami, A.; Kumar, A.; Selvakannan, P.R.; Mandal, S.; Sastry, M.
J Colloid Interface Sci, 2003, **260**(2), 367

33. Phase-transfer of silver nanoparticles from aqueous to organic solutions using fatty amine molecules,
Kumar, A.; Joshi, H.; Pasricha, R.; Mandale, A.B.; Sastry, M.
J Colloid Interface Sci, 2003, **264**(2), 396

34. Magnetic properties of La2MnCo1-xFexO6,
Joly, V.L.; Bhame, S.D.; Joy, P.A.; Date, S.K.
J Magn Magn Mater, 2003, **261**(3), 433

35. Growth of TiO2 nanoparticles in thermally evaporated fatty amine thin films by a method of ion entrapment,
Shankar, S.S.; Rautaray, D.; Pasricha, R.; Pavaskar, N.R.; Mandale, A.B.; Sastry, M.
J Mat Chem, 2003, **13**(5), 1108

36. Bioreduction of chloroaurate ions by geranium leaves and its endophytic fungus yields gold nanoparticles of different shapes,
Shankar, S.S.; Ahmad, A.; Pasricha, R.; Sastry, M.
J Mat Chem, 2003, **13**(7), 1822

37. Ag+-Keggin ion colloidal particles as novel templates for the growth of silver nanoparticle assemblies,
Mandal, S.; Rautaray, D.; Sastry, M.
J Mat Chem, 2003, **13**(12), 3002

38. Biomimetic synthesis of supermagnetic iron-oxide particles in proteins,
Sinha, A.; Nayar, S.; Murthy, G.V.S.;
Joy, P.A.; Rao, V.; Ramachandrarao, P.
J Mat Res, 2003, **18**(6), 1309

39. Development and characterization of novel EPDM/NR prophylactic waste composites,
Mathew, G.; Singh, R.P.; Nair, N.R.; Thomas, S.
J Mat Sci, 2003, **18**(11), 2469

40. A new method for the synthesis of hydrophobic gold nanotapes,
Selvakannan, P.R.; Mandal, S.; Pasricha, R.; Sastry, M.
J Nanosci Nanotechnol, 2003, **3**(5), 372

41. Experimental-evidence to support viscosity dependence of rates of diels-alder reactions in solvent media,
Kumar, A.; Deshpande, S.S.
J Org Chem, 2003, **68**(13), 5411

42. Study of local hard-soft acid-base principle -effects of basis-set, electron correlation, and the electron partitioning method,
Chandrakumar,K.R.S.; Pal,S.
J Phys Chem A, 2003, **107**(30), 5755

43. Ionic interactions from the mixing of NaCl with the acetate, nitrate, perchlorate, and sulfate salts of guanidinium in water,
Kumar, A.
J Phys Chem B, 2003, **107**(12), 2808

44. A novel luminescent functionalized siloxane polymer,
Vinod, M.P.; Bahnemann, D.; Rajamohanan, P.R.; Vijayamohanan, K.;
J Phys Chem B, 2003, **107**(42),11583

45. Effect of chain length and the nature of the monolayer on the electrical behavior of hydrophobically organized gold clusters,
Chaki, N.K.; Aslam, M.; Gopakumar, T.G.; Sharma, J.; Pasricha, R.; Mulla, I.S.; Vijayamohanan, K.
J Phys Chem B, 2003, **107**(49), 13567

46. Multinuclear solid-state MAS/CP-MAS NMR studies of promoter (Phosphate)-enhanced crystallization of Siliceous MCM-41,
Laha, S.C.; Kadgaonkar, M.D.; Anuji, A.; Ganapathy, S.; Amoureux, J.P.; Kumar, R.
J Phys Chem B, 2003, **107**(51), 14171

47. Observation of three different ferromagnetic phases with predictable T(C)s in La2MnCo0.5Ni0.5O6,
Joly, V.L.; Date, S.K.; Joy, P.A.
J Phys Condens Matter, 2003, **15**(14), 243

48. Converting the role of LiClO4 from salting-in to salting-out in Diels-Alder reactions by solvent manipulation,
Deshpande, S.S.; Pawar, S.S.; Phalgune, U.; Kumar, A.
J Phys Org Chem, 2003, **16**(9), 633

49. Self-assembled monolayers of diphenyl disulphide: a novel cathode material for rechargeable lithium batteries,
Maddanimath, T.; Khollam, Y.B.; Aslam, A.;
Mulla, I.S.; Vijayamohanan, K.
J Power Sources, 2003, **124**(1), 133

50. Crystal-structure, magnetic and electrochemical properties of a quaternary thiospinel -Ag2MnSn3S8,
Garg, G.; Ramanujachary, K.V.; Lofland, S.E.; Lobanov, M.V.; Greenblatt, M.; Maddanimath, T.; Vijayamohanan, K.; Ganguly, A. K.
Solid State Chem, 2003, **174**(1), 229

51. SrCO3 crystals of ribbonlike morphology grown within thermally evaporated sodium bis-2-ethylhexylsulfosuccinate thin films,
Rautaray, D.; Sainkar, S.R.; Sastry, M.
Langmuir, 2003, **19**(3), 888

52. Formation of water-dispersible gold nanoparticles using a technique based on surface-bound interdigitated bilayers,
Swami, A.; Kumar, A.; Sastry, M.
Langmuir, 2003, **19**(4), 1168

53. Freely dispersible Au-at-TiO2, Au-at-ZrO2, Ag-at-TiO2 and Ag-at-ZrO2 core shell nanoparticles -one step synthesis, characteri-zation, spectroscopy and optical limiting properties,
Tom, R.T.; Nair, A.S.; Singh, N.; Aslam, M.;
Nagendra, C.L.; Philip, R.; Vijaymohanan, K.; Pradeep, T.
Langmuir, 2003, **19**(8), 3439

54. Capping of gold nanoparticles by the amino acid lysine renders them water-dispersible,
Selvakannan, P.R.; Mandal, S.; Phadtare, S.; Pasricha, R.; Sastry, M. Langmuir, 2003, **19**(8), 3545

55. Extracellular biosynthesis of monodisperse gold nanoparticles by a novel extremophilic actinomycete, Thermomonospora sp.,
Ahmad, A.; Senapati, S.; Khan, M.I.; Kumar, R.; Sastry, M.
Langmuir, 2003, **19**(8), 3550

56. Gold nanoparticles assembled on amine-functionalized Na-Y zeolite: A biocompatible surface for enzyme Immobilization,
Mukhopadhyay, K.; Phadtare, S.; Vinod, V.P.; Kumar, A.; Rao, M.; Chaudhari, R.V.; Sastry, M.
Langmuir, 2003, **19**(9), 3858

57. Investigation into the interaction between surface-bound alkylamines and gold nanoparticles,
Kumar, A.; Mandal, S.; Selvakannan, P.R.; Pasricha, R.; Mandale, A.B.; Sastry, M.
Langmuir, 2003, **19**(15), 6277

58. Time-dependent complexation of cysteine-capped gold nanoparticles with octadecylamine langmuir monolayers at the air-water interface,
Mayya, K.M.; Gole, A.; Jain, N.; Phadtare, S.; Langevin, D.; Sastry, M.
Langmuir, 2003, **19**(22), 9147

59. Studies on the interaction between similarly charged Polyelectrolyte fatty lipid system,
Gole, A.; Phadtare, S.; Sastry, M.; Langevin, D.
Langmuir, 2003, **19**, 9321

60. Ca2+-Keggin anion colloidal particles as templates for the growth of star-shaped calcite crystal assemblies,
Rautaray, D.; Sainkar, S.R.; Sastry, M.
Langmuir, 2003, **19**(24), 10095

61. Investigations on growth mechanism of Poly(O-Anisidine) coatings on low carbon steel by electrochemical synthesis method,
Pawar, P.; Wankhede, M.G.; Patil, P.P.; Sainkar, S.R.
Mat Sci and Engg A -Strut Mat prop microstru, 2003, **347**(1-2), 365

62. Influence of SnO2 over layer on nucleation and growth of diamond films on silicon substrate,
Mahajan, J.R.; More, M.A.; Patil, P.P.; Sainkar, S.R.
Mat Sci and Engg B -solid state Mat Adv Tech, 2003, **97**(2), 117

63. High H2S-sensitive copper-doped tin oxide thin film,
Niranjan, R.S.; Patil, K.R.; Sainkar, S.R.; Mulla, I.S.
Mater Chem Phys, 2003, **80**(1), 250

64. Electrochemical polymerization of 2,5-dimethylaniline on low carbon steel,
Shinde, V.; Chaudhari, S.; Patil, P.P.; Sainkar, S.R.
Mater Chem Phys, 2003, **82**, 622

65. Simple chemical route for the quantitative precipitation of barium-strontium titanyl oxalate precursor leading to Ba1-xSrxTiO3 powders,
Khollam, Y.B.; Bhoraskar, S.V.; Deshpande, S.B.; Potdar, H.S.; Pavaskar, N.R.; Sainkar,
S.R.; Date, S.K.
Mater Lett, 2003, **57**(13-14), 1871

66. Characterization of silicon oxynitride thin-films deposited by electron-beam physical vapor-deposition technique,
Mohite, K.C.; Khollam, Y.B.; Mandale, A.B.; Patil, K.R.; Takwale, M.G.
Mater Lett, 2003, **57**(26-27), 4170

67. Synthesis of nanosized Ce0.75Zr0.25O2 porous Powders via an autoignition: glycine nitrate process,
Potdar, H.S.; Deshpande, S.B.; Khollam, Y.B.; Deshpande, A.S.; Date, S.K.
Mater Lett, 2003, **57**(5-6), 1066

68. Preparation of TiO2 Thin films by modified spin coating methodusing an aqueous precursor,
Patil, K.R.; Sathaye, S.D.; Khollam, Y.B.; Deshpande, S.B.; Pawaskar, N.R.; Mandale, A.B.
Mater Lett, 2003, **57**(12), 1775

69. High performance temperature selective SnO2-Cu-based sensor,
More, P.S.; Khollam, Y.B.; Deshpande, S.B.; Sainkar, S.R.; Date, S.K.; Karekar, R.N.; Aiyer, R.C.
Mater Lett, 2003, **57**(15), 2177

70. Electrochromic materials and devices : Present and future (review),
Somani, P.R.; Radhakrishnan, S.
Mater Phys Chem, 2003, **77**, 117

71. Co-precipitation technique for the preparation of Nanocrystalline ferroelectric SrBi2Ta2O9,
Dhage, S.R.; Kholiam, Y.B.; Deshpande, S.B.; Ravi, V.
Mater Res Bull, 2003, **38**(11-12), 1601

72. Synthesis of ultrafine TiO2 by citrate gel method,
Dhage, S.R.; Pasricha, R.; Ravi, V.
Mater Res Bull, 2003, **38**(11-12), 1623

73. Spin-coated tin oxide -a highly sensitive hydrocarbon sensor,
Niranjan, R.S.; Mulla, I.S.
Mater Sci Eng B-Solid State Mat, 2003, **103**(2), 103

74. Intracellular synthesis of gold nanoparticles by a novel alkalotolerant actinomycete, Rhodococcus species,
Ahmad, A.; Senapati, S.; Khan, M.I.; Kumar, R.; Ramani, R.; Srinivas, V.; Sastry, M.
Nanotechnol, 2003, **14**(7), 824

75. Fractal gold nanostructures produced by the spontaneous reduction of chloroaurate ions in thermally evaporated hexadecylanilinethin films,
Mandal, S.; Phadtare, S.; Selvakannan, P.R.; Pasricha, R.; Sastry, M.
Nanotechnol, 2003, **14**(8), 878

76. Diels-Alder reactions in ionic media: rate enhancement with green chemistry,
Kumar, A.; Deshpande, S.S.; Pawar, S.S.
Natl Acad Sci Lett, 2003, **26**(9-10), 232

77. Uniform CdS quantum dots synthesized in aerosol ot thin films by a process of ion entrapment,
Sivsanker, S.; Sastry, M.
Phys Chem Commun, 2003, **6**, 36

78. Water-dispersible nanoparticles via interdigitation of sodium dodecylsulfate molecules in alkylamine-capped gold nanoparticles at a liquid-liquid interface,
Swami, A.; Jadhav, A.; Kumar, A.; Adyanthaya, S.D.; Sastry, M. Proc Indian Acad Sci, 2003, **115**, 679

79. Lamellar multilayer hexadecylaniline-modified gold nanoparticle films deposited by the langmuir-blodgett technique,
Swami, A.; Kumar, A.; Sastry, M.
Proc Indian Academy of Sciences-Chem, 2003, **115**(3), 185

80. Single-crystal structure, electrical and electrochemical properties of the quaternary thiospinel -Ag2Fesn3S8,
Garg, G.; Gupta, S.; Maddanimath, T.; Gascoin, F.; Ganguli, A.K.
Solid State Ionics, 2003, **164**(3-4), 205

81. Characterization of indium nitride films deposited by activated reactive evaporation process,
Patil, S.J.; Bodas, D.S.; Mandale, A.B.; Gangal, S.A.
Thin Solid Films, 2003, **444**(1-2), 52

Organic chemistry

1. Pyrrolidine carbamate nucleic-acids -synthesis and dna-binding studies,
Meena; Kumar, V.A.
Bioorg Medicinal Chem, 2003, **11**(16), 3393

2. Sulfonate protecting groups. Improved synthesis of scyllo- nositol and its orthoformate from myo-inositol,
Sarmah, M.P.; Shashidhar, M.S.
Carbohyd Res, 2003, **338**(9), 999

3. Towards "designer" surfaces: functionalisation of self-assembled monolayer (SAM) on colloidal gold by alkene metathesis,
Samanta, D.; Faure, N.; Rondelez, F.; Sarkar, A.
Chem Commun, 2003, (10), 1186

4. Expanding the repertoire of pyrrolidyl PNA analogues for DNA/RNA hybridization selectivity: aminoethylpyrrolidinone PNA (Aepone-PNA),
Sharma, N.K.; Ganesh, K.N.
Chem Commun, 2003, (19), 2484

5. Two prolines with a difference: contrasting stereoelectronic effects of 4R/S-aminoproline on triplex stability in collagen peptides [Pro(X)-Pro(Y)-Gly](N),
Umashankara, M.; Babu, I.R.; Ganesh, K.N.
Chem Commun, 2003, (20), 2606

6. Regioselective protection and deprotection of inositol hydroxyl groups,
Sureshan, K.M.; Shashidhar, M.S.; Praveen, T.; Das, T.
Chem Rev, 2003, **103**(11), 4477

7. Sulfonate protecting groups -synthesis of D-myo-Inositol-1,3,4,5 -tetrakisphosphate & L-myo-Inositol-1,3,4,5 -tetrakisphosphate precursors by a novel silver(I) oxide mediated O-alkylation of,
Sureshan, K.M.; Das, T.; Shashidhar, M.S.; Gonnade, R.G.; Bhadbhaade, M.M.
Eur J Org Chem, 2003, (6), 1035

8. Ultrasound promoted acetylation of alcohols in room temperature ionic liquid under ambient conditions,
Gholap, A.R.; Venkatesan, K.; Daniel, T.; Lahoti, R.J.; Srinivasan, K.V. Green Chem, 2003, **5**(6), 693

9. Solid acid catalysts for fluorotoluene nitration using nitric acid,
Maurya, S.K.; Gurjar, M.K.; Malshe, K.M.; Patil, P.T.; Dongare, M.K.; Kemnitz, E. Green Chem,
2003, **5(6),** 720

10. Synthesis of rigid bicycloheterocyclic scaffolds from Vince's lactam (enzymatic resolution of vince's lactam),
Gurjar, M.K.; Bera, S.; Joshi, R.R.; Joshi, R.A.
Heterocycles, 2003, **60**(10), 2293

11. Chiral 1,3-oxazolidines as the ligands for the enantioselective addition of diethylzinc to aryl Aldehydes,
Prasad, K.R.; Joshi, N.N.
Indian J Chem B, 2003, **42**(1), 150

12. Ligands and Ru catalysts, Ru DAB, Salen and DMSO complexes catalyzed selective transfer hydrogenation of ketones and aldehydes,
Iyer, S.; Sattar, A.K.
Indian J Chem B, 2003, **42**(11), 2805

13. Alkali cleavage of α,α-disubstituted β-ketoesters, nitriles and β-diketones,
Bennur, T.H.; Joshi, N.N.
Indian J Chem B, 2003, **42**(3), 670

14. Ionic liquid-promoted regiospecific friedlander annulation: novel synthesis of quinolines and fused polycyclic quinolines,
Palimkar, S.S.; Siddiqui, S.A.; Daniel, T.; Lahoti, R.J.; Srinivasan, K.V.
J Org Chem, 2003, **68** (24), 9371

15. N7-Guanine as a C+ mimic in hairpin Aeg/aeppna - DNA triplex -probing binding selectivity by UV-T-M and kinetics by flurescence based strand invasion assay,
Dcosta, M.; Kumar, V.A.; Ganesh, K.N.
J Org Chem, 2003, **68**(11), 4439

16. Truly catalytic and enantioselective pinacol coupling of aryl aldehydes mediated by chiral Ti(III) complexes,
Chatterjee, A.; Bennur, T.H.; Joshi, N.N.
J Org Chem, 2003, **68**(14), 5668

17. Enantioselective synthesis of L-CCG-I,
Chavan, S.P.; Sharma, P.; Sivappa, R.; Bhadbhade, M.M.; Gonnade, R.G.; Kalkote, U.R.
J Org Chem, 2003, **68**(17), 6817

18. A rational study of crystal engineering of supramolecular assemblies of 1,2,4,5-benzenetetracarboxylic acid,
Arora, K.K.; Pedireddi, V.R.
J Org Chem, 2003, **68**(24), 9177

19. Synthesis and structure of novel, air-stable carbyne complexes of Tungsten,
Hazra, D.; Sinhmahapatra, D.K.; Puranik, V.G.; Sarkar, A.
J Organometallic Chem, 2003, **671**(1-2), 52

20. New synthesis of 1-aryl-4-(4-hydroxy-3,5-diiodo-α-methylbenzylidene)-2-phenylimidazol-5-ones,
Bhusare, S.R.; Shekapure, J.L.; Pawar, R.P.; Vibhute, Y.B.; Bhawal, B.M.
Khimiya Geterotsiklicheskikh Soedinenii, 2003, (6), 853

21. Structural pre-organization of peptide nucleic-acids
Kumar, V.A.,
Nucleosides Nucleotides Nucleic Acids, 2003, **22**(5-8), 1045

22. Pyrrolidine pna-dna chimeric oligonucleotides with extended backbone,
Kumar, V.A.; Meena
Nucleosides Nucleotides Nucleic Acids, 2003, **22**(5-8), 1101

23. Piperidinyl peptide nucleic - acids -synthesis and dna-complementation studies,
Lonkar, P.; Kumar, V.A.;
Nucleosides Nucleotides Nucleic Acids, 2003, **22**(5-8), 1105

24. Synthesis of trans-l/d-2-(tert-butoxycarbonyl-aminomethyl)-4-(thymin-1-yl) pyrrolidin-1-yl acetic-acid,
Kumar, V.A.; Meena
Nucleosides Nucleotides Nucleic Acids, 2003, **22**(5-8), 1285

25. Chelation control in nucleophilic addition to Cr(CO) (3) complexed aryl aldehydes,
Tipparaju, S.K.; Puranik, V.G.; Sarkar, A.
Org Biomol Chem, 2003, **1**(10), 1720

26. A new access to polyhydroxy piperidines of the azasugar class -synthesis and glycosidase inhibition studies,
Pandey, G.; Kapur, M.; Khan, M.I.; Gaikwad, S.M.
Org Biomol Chem, 2003, **1**(19), 3321

27 Synthesis of spirocycles via ring closing metathesis of heterocycles carrying gem-diallyl substituents obtained via ring opening of (Halomethyl) cyclopropanes with allyltributyltin,
Gurjar, M.K.; Ravindranadh, S.V.; Sankar, K.; Karmakar, S.; Cherian, J.; Chorghade, M.S.
Org Biomol Chem, 2003, **1**(8), 1366

28. Evidence for the involvement of silver nanoclusters during the wolff rearrangement of α-diazoketones,
Sudrik, S.G.; Maddanimath, T.; Chaki, N.K.; Chavan, S.P.; Sonawane, H.R.; Vijayamohanan, K.
Org Lett, 2003, **5**(13), 2355

29. (1S,2R/1R,2S)-Aminocyclohexyl glycyl thymine PNA - synthesis, monomer crystal-structures, and DNA/RNA hybridization studies,
Govindaraju, T.; Gonnade, R.G.; Bhadbhade, M.M.; Kumar, V.A.; Ganesh, K.N.
Org Lett, 2003, **5**(17), 3013

30. NaIO(4)-mediated selective oxidative halogenation of alkenes and aromatics using alkali metal halides,
Dewkar, G.K.; Narina, S.V.; Sudalai, A.
Org Lett, 2003, **5**(23), 4501

31. Transition-metal-catalyzed regio-selective and stereoselective aminobromination of olefins with TSNH 2 and NBS as nitrogen and bromine sources,
Thakur, V.V.; Talluri, S.K.; Sudalai, A.
Org Lett, 2003, **5**(6), 861

32. Anomeric configuration-directed diastereoselective C-C bond formation in vinyl sulfone-modified carbohydrates: A general route to branched-chain sugars,
Sanki, A.K.; Suresh, C.G.; Falgune, U.D.; Pathak, T.
Org Lett, 2003, **5**(8), 1285

33. A short synthesis of Ar-todomatuic acid and dihydro-Ar-turmerone by the heck reaction,
Solabannavar, S.B.; Wadgaonkar, P.P.; Desai, U.V.; Mane, R.B.
Org Prep Proced Int, 2003, **35**(4), 418

34. A new route to prepare 6-chloro-5-(2-chloroethyl) oxindole,
Gurjar, M.K.; Murugaiah, A.M.; Reddy, D.S.; Chorghade, M.S.
Org Process Res Dev, 2003, **7**(3), 309

35. Isolation and X-ray study of an antiinflammatory active andostene steroid from acacia nilotica,
Chaubal, R.; Mujumdar, A.M.; Puranik, V.G.; Deshpande, V.H.; Deshpande, N.R.
Planta Medica, 2003, **69**(3), 287

36. Magnesium/methanol,
Pasupathy, K.
Synlett, 2003, (12), 1942

37. Pyrrolidine-2-carboxylic acid (L-proline),
Paraskar, A.S.
Synlett, 2003, (4), 582

38. PCC: Novel oxidation reactions,
Fernandes, R.A.
Synlett, 2003, (5), 741

39. Enantioselective syntheses of xylo-C-18-phytosphingosines using double stereodifferentiation,
Fernandes, R.A.; Kumar, P.
Synthesis Stutt, 2003, (1), 129

40. Synthesis of marine natural product (2S,5S)-pyrrolidine-2,5-dicarboxylic acid,
Sunilkumar, G.; Nagamani, D.; Argade, N.P.; Ganesh, K.N.
Synthesis Stutt, 2003, (15), 2304

41. A simple and efficient method for transesterification of β–ketoesters catalysed by iodine,
Chavan, S.P.; Kale, R.R.; Shivasankar, K.; Chandake, S.I.; Benjamin, S.B.
Synthesis Stutt, 2003, (17), 2695

42. An easy access to (E)-alkylidenesuccinic acids,
Mangaleswaran, S.; Argade, N.P.
Synthesis Stutt, 2003, (3), 343

43. Facile routes to alkoxymaleimides / maleic anhydrides,
Sahoo, M.K.; Mhaske, S.B.; Argade, N.P.
Synthesis Stutt, 2003, (3), 346

44. New route for the synthesis of (22S, 23S)-28-homobrassinolide,
Massey, A.P.; Pore, V.S.; Hazra, B.G.
Synthesis Stutt, 2003, (3), 426

45. Base-induced alcoholysis of N-arylmaleimides: Facile in situ oxa-michael addition to alkyl maleanilates: Two-step one-pot rapid access to alkoxysuccinic acids,
Mhaske, S.B.; Argade, N.P.
Synthesis Stutt, 2003, (6), 863

46. Simple synthesis of two naphthoquinone antibiotics psychorubrinand pentalongin,
Bulbule, V.J.; Koranne, P.S.; Munot, Y.S.; Borate, H.B.; Deshpande, V.H.
Synthetic Commun, 2003, **33**(4), 587

47. Synthesis of a few bis-binaphthol derivatives,
Jha, S.C.; Joshi, N.N.
Synthetic Commun, 2003, **33**(6), 1005

48. A facile deprotection of dithioacetals by FeCl3/KI,
Chavan, S.P.; Soni, P.B.; Kale, R.R.; Pasupathy, K.
Synthetic Commun, 2003, **33**(6), 879

49. Regio-selective mono nitration of phenols with ferric nitrate in room temperature ionic liquid,
Rajagopal, R.; Srinivasan, K.V.
Synthetic Commun, 2003, **33**(6), 961

50. An efficient Co(II) catalyzed auto oxidation of 1,4-dihydropyridines,
Chavan, S.P.; Kharul, R.K.; Kalkote, U.R.; Shivakumar, I.
Synthetic Commun, 2003, **33**(8), 1333

51. Studies on bromination of active methylene by a mixture of hydrobromic acid and hydrogen peroxide (Or TBHP),
Tillu, V.H.; Shinde, P.D.; Bedekar, A.V.; Wakharkar, R.D.
Synthetic Commun, 2003, **33**(8), 1399

52. 4-Formylazetidin-2-ones, synthon for the facile synthesis of enantiopure 4-aminopiperidin-2-ones,
Krishnaswamy, D.; Govande, V.V.; Rakeeb, A.; Deshmukh, A.S.
Synth-Stutt, 2003, (12), 1903

53. A novel and simple asymmetric synthesis of CMI-977 (LDP-977): a potent anti-asthmatic drug lead,
Gurjar, M.K.; Murugaiah, A.M.; Radhakrishna, P.; Ramana, C.V.; Chorghade, M.S.
Tetrahedron Asymmetry, 2003, **14**(10), 1363

54. Amano PS-catalysed enantioselective acylation of (+/-)-α-methyl-1,3-benzodioxole-5-ethanol: an efficient resolution of chiral intermediates of the remarkable antiepileptic drug candidate,
Easwar, S.; Argade, N.P.
Tetrahedron Asymmetry, 2003, **14**(3), 333

55. WO3-30% H2O2-Cinchona alkaloids: A new heterogeneous catalytic system for the asymmetric oxidation of sulfides and the kinetic resolution of racemic sulfoxides,
Thakur, V.V.; Sudalai, A.
Tetrahedron Asymmetry, 2003, **14**(4), 407

56. Ephedrine derived reusable chiral auxiliary for the synthesis of optically pure 3-hydroxy-4-aryl-β-lactams,
Shinkre, B.A.; Puranik, V.G.; Bhawal, B.M.; Deshmukh, A.R.
Tetrahedron Asymmetry, 2003, **14**(4), 453

57. Enantioselective synthesis of (R)-(-)-baclofen via Ru(II)-BINAP catalyzed asymmetric hydrogenation,
Thakur, V.V.; Nikalje, M.D.; Sudalai, A.
Tetrahedron Asymmetry, 2003, **14**(5), 581

58. Total synthesis of microcarpalide,
Gurjar, M.K.; Nagaprasad, R.; Ramana, C.V.
Tetrahedron Lett, 2003, **44**(14), 2873

59. I-2 As an efficient catalyst in ionic Diels-Alder reactions of α,β- unsaturated acetals,
Chavan, S.P.; Sharma, P.; Krishna, G.R.; Thakkar, M.
Tetrahedron Lett, 2003, **44**(14), 3001

60. Cu(OTf)(2): a reusable catalyst for high-yield synthesis of 3,4- dihydropyrimidin-2(1H)-ones,
Paraskar, A.S.; Dewkar, G.K.; Sudalai, A.
Tetrahedron Lett, 2003, **44**(16), 3305

61. A novel intramolecular arene-alkene photocycloaddition in 2- alkenyl naphtha-4-chromanones -a short route to functionalized multicyclic systems,
Kalena, G.P.; Pradhan, P.; Puranik, V.S.; Banerji, A.
Tetrahedron Lett, 2003, **44**(19), 2011

62. An asymmetric dihydroxylation route to (S)-oxybutynin,
Gupta, P.; Fernandes, R.A.; Kumar, P.
Tetrahedron Lett, 2003, **44**(22), 4231

63. Total-synthesis of cis and trans-hydroxyglimepiride - active metabolite of glimepiride,
Gurjar, M.K.; Joshi, R.A.; Chaudhuri, S.R.; Joshi, S.V.; Barde, A.; Gediya, L.K.; Ranade, P.V.; Kadam, S.M.; Naik, S.J.
Tetrahedron Lett, 2003, **44**(26), 4853

64. A novel additive organic supramolecular assembly - molecular-complex of 3,5-dinitrobenzamide and 3,5-dinitrobenzonitrile,
Pedireddi, V.R.; Prakashareddy, J.; Arora, K.K.
Tetrahedron Lett, 2003, **44**(26), 4857

65. Synthesis of novel chiral spirodione, (6r,7r)-7-phenyl-1 oxaspiro(5.5)undec-3-ene-2,5-dione -application to the asymmetric diels-alder reaction with high pi-facial selectivity,
Kandula, S.V.; Puranik, V.G.; Kumar, P.
Tetrahedron Lett, 2003, **44**(27), 5015

66. Carbohydrate-based synthesis of crocacin - stereoselective heck reaction of carbohydrate 5,6-ene-derivative and 5,6-yne-derivative with aromatic halides,
Gurjar, M.K.; Khaladkar, T.P.; Borhade, R.G.; Murugan, A.
Tetrahedron Lett, 2003, **44**(28), 5183

67. Asymmetric-synthesis of (-)-acaterin,
Kandula, S.R.V.; Kumar, P.
Tetrahedron Lett, 2003, **44**(32), 6149

68. Study of the reactivity profile of glycine schiffs bases with dipolarophiles -application towards a concise synthesis of CCG-II (Vol 37, Pg 2857, 1996),
Chavan, S.P.; Venkatraman, M.S.; Sharma, A.K.; Chittiboyina, A.G.
Tetrahedron Lett, 2003, **44**(32), 6173

69. Enantioselective synthesis of (r)-phenylephrine hydrochloride,
Pandey, R.K.; Upadhyay, P.K; Kumar, P.
Tetrahedron Lett, 2003, **44**(33), 6245

70. Supramolecular Pseudopolymorphs -Double Helix and Planar Structures with Channels,
Pedireddi, V.R.; Prakashareddy, J.
Tetrahedron Lett, 2003, **44**(35), 6679

71. Enantioselective synthesis of D-ribo-(2S,3S,4R)-C-18-phytosphingosine using double stereodifferentiation,
Naidu, S.V.; Kumar, P.
Tetrahedron Lett, 2003, **44**(5), 1035

72. N-bromoamides as versatile catalysts for aziridination of olefins using chloramine-T,
Thakur, V.V.; Sudalai, A.
Tetrahedron Lett, 2003, **44**(5), 989

73. PCC-mediated novel oxidation reactions of homobenzylic and homoallylic alcohols,
Fernandes, R.A.; Kumar, P.
Tetrahedron Lett, 2003, **44**(6), 1275

74. Lipase catalyzed polyster synthesis in 1-butyl-3-methylimidazolium hexafluorophosphate ionic liquid,
Nara, S.J.; Harjani, J.R.; Salunkhe, M.M.; Mane, A.T.; Wadgaonkar, P.P.
Tetrahedron Lett, 2003, **44**(7), 1371

75. Ionic liquid promoted regioselective monobromination of aromatic substrates with N-bromosuccinimide,
Rajagopal, R.; Jarikote, D.V.; Lahoti, R.J.; Daniel, T.; Srinivasan, K.V.
Tetrahedron Lett, 2003, **44**(9), 1815

76. Diastereospecific synthesis of novel [3.6.6.4.7]-fused pentacyclic β-lactams by 6-exo-trig, 7-endo-dig tandem radical cyclization,
Joshi, S.N.; Phalgune, U.D.; Bhawal, B.M.; Deshmukh, A.R.
Tetrahedron Lett, 2003, **44**(9), 1827

77. Room temperature ionic liquid promoted synthesis of 1,5-benzodiazepine derivatives under ambient conditions,
Jarikote, D.V.; Siddiqui, S.A.; Rajagopal, R.; Daniel, T.; Lahoti, R.J.; Srinivasan, K.V.
Tetrahedron Lett, 2003, **44**(9), 1835

78. Enantioselective synthesis of (-) -α-conhydrine via cyclic sulfate methodology,
Kandula, S.V.; Kumar, P.
Tetrahedron Lett, 2003, **44**(9), 1957

79. 1st Synthesis of Aza-calanolides -A new class anti-HIV active compounds,
Sharma, G.V.M.; Jiagovan, A.; Narayanan, V.L.; Gurjar, M.K.
Tetrahedron, 2003, **59**(1), 95

80. Facile synthesis of meso-substituted dipyrromethanes and porphyrins using cation exchange resins,
Naik, R.; Joshi, P.; Kaiwar, S.P.; Deshpande, R.K.
Tetrahedron, 2003, **59**(13), 2207

81. Asymmetric synthesis of azetidin-2-ones by [2+2] cycloaddition using chiral imines derived from D-(+)-glucose,
Arun, M.; Joshi, S.N.; Puranik, V.G.; Bhawal, B.M.; Deshmukh, A.R.
Tetrahedron, 2003, **59**(13), 2309

82. An efficient synthesis of (+/-)-β-herbertenol by a 1,3-cyclopentadione annelation strategy,
Chavan, S.P.; Kharul, R.K.; Kale, R.R.; Khobragade, D.A.
Tetrahedron, 2003, **59**(15), 2737

83. A facile access to natural and unnatural dialkyl substituted maleic anhydrides,
Kar, A.; Argade, N.P.
Tetrahedron, 2003, **59**(17), 2991

84. Enantioselective synthesis of pantolactone analogues from an ephedrine-derived morpholine-dione,
Pansare, S.V.; Bhattacharyya, A.
Tetrahedron, 2003, **59**(18), 3275

85. Salt effects on the Baylis-Hillman reaction,
Kumar, A.; Pawar, S.S.
Tetrahedron, 2003, **59**(27), 5019

86. N-Bromosuccinimide-dibenzoyl peroxide/ azabisisobutyronitrile -A reagent for Z-alkene to E-alkene isomerization,
Baag, M.; Kar, A.; Argade, N.P.
Tetrahedron, 2003, **59**(34), 6489

87. Synthesis of anomerically pure vinyl sulfone-modified pent-2-enofuranosides and hex-2-enopyranosides -a group of highly reactive michael acceptors for accessing carbohydrate-based synthons,
Sanki, A.K.; Pathak, T.
Tetrahedron, 2003, **59**(36), 7203

88. Ultrasound promoted para-selective nitration of phenols in ionic liquid,.
Rajagopal, R.; Srinivasan, K.V.
Ultrason Sonochemistry, 2003, **10**(1), 41

89. Ultrasound promoted facile synthesis of arylhydrazones at ambient conditions,
Jarikote, D.V.; Deshmukh, R.R.; Rajagopal, R.; Lahoti, R.J.; Daniel, T.; Srinivasan, K.V.
Ultrason Sonochemistry, 2003, **10**(1), 45

Polymer sciences

1. Biodegradation of poly(ε-caprolactone)/starch blends and composites in composting and culture environments: the effect of compatibilization on the inherent biodegradability of the host polymer,
Singh, R.P.; Pandey, J.K.; Rutot, D.; Degee, P.; Dubois, P.
Carbohyd Res, 2003, **338**(17), 1759

2. Sensitizarion effect in doped and undoped state of polypyrrole by methylene blue in solid state electrochemical cells,
Somani, P.R.; Radhakrishnan, S.
Chem Phys Lett, 2003, **379**, 401

3. Telechelic cis-1,4-oligoisoprene through the selective oxidolysis of epoxidized monomer units and polyisoprenic monomer units in cis-1,4-polyisoprenes,
Gillier-Ritoit, S.; Reyx, D.; Campistron, I.; Laguerre, A.; Singh, R.P.
J Appl Polym Sci, 2003, **87**(1), 42

4. Thermal decomposition kinetics of photooxidized nylon 66,.
Singh, R.P.; Desai, S.M.; Pathak, G.
J Appl Polym Sci, 2003, **87**(13), 2146

5. Preparation and characterization of poly (methyl methacrylate) clay nanocomposites via melt intercalation -The effect of organoclay on the structure and thermal properties,
Kumar, S.; Jog, J.P.; Natarajan, U.
J Appl Polym Sci, 2003, **89**(5), 1186

6. Polymorphism in intercalated poly(vinylidene fluoride)/clay nanocomposites,
Priya, C.; Jog,J.P.
J Appl Polym Sci, 2003, **89**(8), 2036

7. Effect of modified layered silicates and compatibilizer on properties of PMP/clay nanocomposites,
Wanjale, S.D.; Jog, J.P.
J Appl Polym Sci, 2003, **90**(12), 3233

8. Ecofriendly behavior of host matrix in composites prepared from agro-waste and polypropylene,
Pandey, J.K.; Ahmad, A.; Singh, R.P.
J Appl Polym Sci, 2003, **90**(4), 1009

9. Synthesis of new polymeric hindered amine light stabilizers -performance evaluation in styrenic polymers,
Singh, R.P.; Patwa, A.N.; Desai, S.M.; Pandey, J.K.; Solanky, S.S.; Prasad, A.V.
J Appl Polym Sci, 2003, **90**(4), 1126

10. Revisiting emulsion polymerization to produce stable, translucent, nanolatex of partially water soluble monomers, ethylacrylate -methacrylate,
Bhawal, S.; Dhoble, D.; Surekha, D.
J Appl Polym Sci, 2003, **90**, 2593

11. Poly (1-butene)/clay nanocomposites: A crystallization study,
Wanjale, S.D.; Jog, J.P.
J Macromol Sci Phys, 2003, **B42**(6), 1141

12. Crystallization and melting behavior of polypropylene in presence of hydrogenated dicyclopentadiene,
Wanjale, S.D.; Priya, L.; Jog, J.P.
J Macromol Sci-Phys, 2003, **B42**(5), 1007

13. Preparation and characterization of polyketone/clay nanocomposites,
Bulakh, N.; Kulkarni, S.M.; Jog, J.P.; Chaudhari, R.V.;
J Macromol Sci-Phys, 2003, **B42**(5), 963

14. Theoretical calculation of the optical anisotropy of substituted cyclohexanes and associated bisphenyl molecules using experimentally derived group polarizabilities,
Sulatha, M.S.; Sivaram, S.; Natarajan, U.
J Phys Chem A, 2003, **107**(1), 97

15. Structural changes in semicrystalline poly(ether ester) on UV irradiation,
Sarwade, B.D.; Singh, R.P.
J Polym Eng, 2003, **23**(1), 43

16. Intercalated poly(vinylidene fluoride)/clay nanocomposites: structure and properties,
Priya, L.; Jog, J.P.
J Polym Sci B -Polym Phys, 2003, **41**(1), 31

17. Poly(1-butene)/clay nanocomposites: Preparation and properties,
Wanjale, S.D.; Jog, J.P.
J Polym Sci B -Polym Phys, 2003, **41**(10), 1014

18. New interpretation of progression bands observed in Infrared spectra of nylon -M/N,
Yoshioka, Y.; Tashiro, K.; Ramesh, C.
J Polym Sci B -Polym Phys, 2003, **41**(12), 1294

19. Copolyester/layered silicate nanocomposites: The effect of the molecular size and molecular structure of the intercalant on the structure and viscoelastic properties of the nanocomposites,
Kalgaonkar, R.A.; Jog, J.P.
J Polym Sci B -Polym Phys, 2003, **41**(23), 3102

20. Functional group determination in controlled chain-cleaved natural rubber,
Solanky, S.S.; Campistron, I.; Singh, R.P.
J Rubber Res, 2003, **6**, 1

21. Effect of LiClO4 and LiCl additives on the kinetics of anionic- polymerization of methyl-methacrylate in toluene- tetrahydrofuran mixed-solvent,
Dhara, M.G.; Baskaran, D.; Sivaram, S.
Macromol Chem Phys, 2003, **204**(12), 1567

22. Biodegradation of packaging materials : Composting of polyolefins,
Singh, R.P.; Pandey, J.K.; Pratheepkumar, A.
Macromol Symposia, 2003, **197**, 411

23. Copolyesters based on poly(Butylene terephthalate)s containing cyclohexyl groups: Synthesis, structure and crystallization,
Sandhya, T.E.; Ramesh, C.; Sivaram, S.
Macromol Symposia, 2003, **199**, 467

24. RIS models and unperturbed chain properties of polyesters containing 1,3-cyclobutylene and 1,4-cyclohexylene linkages,
Sulatha, M.S.; Natarajan, U.
Macromol Theory Simul, 2003, **12**(1), 61

25. Optical anisotropy of structurally modified polycarbonates having cyclohexylidene and methyl substituents using the rotational isomeric state method,
Sulatha, M.S.; Sivaram, S.; Natarajan, U.
Macromolecules, 2003, **36**(8), 2944

26. Studies on the Clathrate (δ) form of syndiotactic polystyrene crystallized by different solvents using Fourier transform infrared spectroscopy,
BhojeGowd, E.; Nair, S.S.; Ramesh, C.; Tashiro, K.
Macromolecules, 2003, **36**, 7388

27. Solid polymer electrolyte with methylene blue and its thermal properties,
Somani, P.S.; Radhakrishnan, S.
Polym Degrad Stab, 2003, **79**, 77

28. Transport of aromatic solvents through nitrile rubber/ epoxidized natural rubber blend membranes,
Mathai, A.E.; Singh, R.P.; Thomas, S.
Polym Engg and Sci, 2003, **43**(3), 704

29. Effect of fluorene-bisphenol ring substitution and bridge rigidity on physical and gas permeation properties of resulting polyarylates,
Bhole, Y.S.; Kharul, U.K.
Polym Int, 2003, **52**(9), 1474

30. Structural-change in the brill transition of nylon M/N (2) conformational disordering as viewed from the temperature-dependent infrared spectral measurements,
Yoshioka, Y.; Tashiro, K.; Ramesh, C.
Polymer, 2003, **44**(20), 6407

31. Controlled grafting of N-isoproply acrylamide brushes onto self-standing isotactic polypropylene thin films: surface initiated atom transfer radical polymerization,
Desai, S.M.; Solanky, S.S.; Mandale, A.B.; Rathore, K.; Singh, R.P.
Polymer, 2003, **44**(25), 7645

32. Hyperbranched polymers from divinylbenzene and 1,3-diisopropenylbenzene through anionic self condensing vinyl polymerization,
Baskaran, D.
Polymer, 2003, **44**(8), 2213

33. Strategic developments in living anionic-polymerization of alkyl(methyl) acrylates,
Baskaran, D.
Progress in Polym Sci, 2003, **28**(4), 521

34. A study of the utilization of reclaimed natural rubber prophylactic in blend with epoxidized natural rubber and silica,
Mathew, G.; Singh, R.P.; Groeninckx, G.; Thomas, S.
Progress in Rubber, plastics Recycl Technol, 2003, 205

35. Study of heavy-ion modified Cr-39 (diethyleneglycol bisallyl carbonate),
Srivastava, A.; Singh, T.; Sharma, A.L.; Jain, P.K.; Ponrathnam, S.; Rajan, C.R.
Radiat Eff Defect Solids, 2003, **158**(8), 561

36. The Mukaiyama-Michael addition of a β,β-dimethyl substituted silyl ketene acetal to α,β-unsaturated ketones using tetra-N-butylammonium bibenzoate as a nucleophilic catalyst,
Gnaneshwar, R.; Wadgaonkar, P.P.; Sivaram, S.
Tetrahedron Lett, 2003, **44**(32), 6047

Foreign patents granted (2003)

	Title	Inventor (s)	Country (Patent No.)
1	An improved process for the preparation of thiourea	Balakrishnan, S., Mahajan, S.S., Chaphekar, G.M., Gupte, M.Y., Kulkarni, M.P., Krishnamurthy, B.P.R.	US 6,657,082
2	A process for the preparation of poly (ester-carbonate)s	Hait, S.B., Sivaram, S.	EP 908483
3	Strain of streptomyces for the preparation of an alkaline protease inhibitor	Vernekar, J.V., Ghatge, M.S., Rao, M.B., Deshpande, V.V.	US 6,514,748
4	Low temperature process for the production of hydrogen	Choudhary, V.R., Rajput, A.M., Banerjee, S.	US 6,509,000
5	Mifepristone analogue, process for the preparation thereof and use thereof (NCL-CDRI, Lucknow)	Hazra, B.G., Pore, V.S., Joshi, P.L., Basu, S., Singh, J., Dwivedi, A.	US 6,512,130
6	A process for the preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst	Choudhary, V.R., Jana, S.K.	US 6,548,722
7	Thermoprecipitating polymer containing enzyme specific ligands, process for the preparation thereof, and process for the separation of enzymes using such polymers	Vaidya, A.A., Lele, B.S., Kulkarni, M.G., Mashelkar, R.A.	US 6,605,714
8	Process for the activation of a metallic palladium based catalyst useful for the direct oxidation of hydrogen to hydrogen peroxide	Choudhary, V.R., Gaikwad, A.G., Sansare, S.D.	US 6,534,440
9	Noble metal containing hydrogenation catalyst for the selective hydrogenation of 1,4 butynediol to 1,4 butenediol and a process for the preparation thereof	Chaudhari, R.V., Rode, C.V., Jaganathan, R., Telkar, M.M., Rane, V.H.	US 6,660,675
10	Process for treatment of mixture of spent wash from distillery and black liquor from pulp and paper industry	Moghe, P.P., Panchanadikar, V.V., Pol, A.V., Joshi, A.R., Bahirat, P.K., Kudlu, P., Bahirat, S.P.	US 6,589,427
11	Process for the preparation of acetic acid or methyl acetate	Kelkar, A.A., Tonde, S.S., Divekar, S.S., Chaudhari, R.V.	US 6,521,784
12	Process for the preparation of acidic lipase	Mahadik, N.D., Gokhale, D.V., Bastawde, K.B., Khire, J.M., Puntambekar, U.S.	US 6,534,303
13	Process for the preparation of a nanosized colloidal metal particle	Mukherjee, P., Mandal, D., Ahmad, A., Murali Sastry,Rajiv Kumar,	US 6,537,344
14	Process for the preparation of 1-[cyano (aryl) methyl] cyclohexanol	Chavan, S.P., Kamat, S.K., Sivadasan, L., Balakrishnan, K., Khobragade, D.A., Ravindranathan, T., Gurjar, M.K., Kalkote, U.R.	US 6,504,044

	Title	Inventor (s)	Country (Patent No.)
1	Process for the preparation of an aromatic carboxylic acid	Srinivas, D., Chavan, S.A., Ratnasamy, P.	US 6,649,791
2	A process for the preparation of phenyl ketones	Chidambaram, M., Venkatesan, C., Singh, A.P., Ramaswamy, A.V.	US 6,593,499
3	Tinuvin P-hindred amine light stabilizer and derivatives thereof	Singh, R.P., Desai, S.M.	US 6,610,856 (Divisional of 6,492,518)
4	Noble metal containing hydrogenation catalyst for selective hydrogenation of 1,4-butynediol to 1,4 butenediol, and a process for the preparation thereof	Chaudhari, R.V., Rode, C.V., Jaganathan, R., Telkar, M.M., Rane, V.H.	US 6,528,689
5	Process for the synthesis of a photo-stabilizer	Desai, S.M., Singh, R.P.	US 6,559,311
6	Process for preparation of a lactone from a cyclic ketone	Mandal, D., Ahmad, A., Khan, M.I., Rajiv Kumar,	US 6,559,322
7	Process for the preparation of adipic acid	Srinivas, D., Chavan, S.A., Ratnasamy, P.	US 6,521,789
8	Process for the preparation of 2-aryl propionic acids	Chaudhari, R.V., Seayad, J., Seayad, A.	US 6,660,883
9	Composition for hybrid seed production, process for the preparation of such composition and use thereof	Mahajan, V., Nagarajan, S., Deshpande, V.H., Kelkar, R.G., Lahoti, R.J., Ramlingam, S., Bulbule, V.J.	US 6,645,917
10	Process for the preparation of alkyl 4[2-(phthalimido)ethoxy]-acetoacetate	Joshi, R.R., Joshi, R.A., Ravindranathan, T.	US 6,562,983
11	Process for the preparation of 2-acrylamido-2-methyl-1-propanesulfonic acid	Barve, P.P., Joshi, S.S., Shinde, R.W., Gupte, M.Y., Joshi, C.N., Ghike, S.M., Naik, R.V., Kulkarni, R.A., Bote, A.N.	US 6,504,050
12	Process for the preparation of 2-Methyl-2-Propene-1-Sulfonic acid, Sodium salt	Barve, P.P., Joshi, S.S., Shinde, R.W., Ghike, S.M., Gupte, M.Y., Joshi, C.N., Naik, R.V.	US 6,660,882
13	Process for making S(-) Amlodipine salts	Joshi, R.R., Joshi, R.A., Gurjar, M.K.	US 6,608,206
14	Process for preparation of substituted aromatic compound employing Friedel-Crafts reaction using a reusable basic anionic clay catalyst	Choudhary, V.R., Jana, S.K.	US 6,525,226

Indian patents granted (2003)

	Title	Inventor	Patent No.
1	A process for the preparation of Ankle Block component useful for artificial foot	Nadkarni, V.M., Pandit, S.B., Patil, P.S., Rajan, C.R.	187915
2	An improved process for the preparation of polyester polyol useful for the preparation of the ankle block component of the artificial foot	Nadkarni, V.M., Vaidya, U.R., Pandit, S.B., Patil, P.S., Rajan, C.R.	187914
3	An improved process for the preparation of grinding wheels made thereby	Nadkarni, V.M., Ayodhya, S.R., Rajan, C.R.	188035
4	An improved process for the separation of Dihydroxybenzene isomers using zeolite LTL	Moghe, P.P,Bahirat, P.K., Joshi, P.N., Shiralkar, V.P., Biswas, S.S.	188181
5	A process for the preparation of polyalkylene terephthalate containing at least 3 carbon atoms from polyethylene terephthalate (PET) waste useful as an engineering thermoplastic	Sivaram, S., Avadhani, C.V.	187889
6	An improved process for the preparation of Caprolactam	Jha, B.K., Chhatre, A.S., Kulkarni, B.D., Shivasanker, S.,	189045
7	An improved process for the preparation of polymer containing metal composite materials	Nadkarni, V.M., Rajan, C.R., Ayodhya, S.R.	188894
8	An improved process for the preparation of polymer containing ceramic composites materials	Nadkarni, V.M., Ayodhya, S.R., Rajan, C.R.	189146
9	An improved process for the preparation of Esters from carboxylic acids and alcohols using Zeolite catalyst	Bhawal, B.M., Deshmukh, A.R.A.S., Gumaste, V.K., Shiralkar, V.P., Rao, B.S.	188532
10	An improved process for the preparation of N-Acetyl amino phenol	Gopinathan, C., Gopinathan, S., Kuruvilla, J., Pardhy, S.A., Ratnasamy,	189140
11	An improved process for the preparation of an improved supported catalyst useful for oxidative conversion of methane, natural gas and biogas to synthetic gas	Uphade, B.S., Mamman, A.S., Rajput, A.M., Choudhary, V.R.	189145
12	A process for the preparation of a compound containing urethane linkage useful as plasticizer for polyvinylchloride (PVC)	Srinivasan, S.R., Raut, K.G., Saxena, P.K., Sivaram,	188825
13	A process for the preparation of improved compounded poly(vinylchloride) (PVC)	Srinivasan, S.R., Raut, K.G., Saxena P.K., Sivaram,	188046
14	An improved process for the preparation of Monochlorophthalic anhydride	Kuruvilla, J., Gopinathan, C., Gopinathan, S., Pardhy, S.A., Ratnasamy, p.,	188690
15	An improved process for the preparation of aromatic aldehydes	Kuruvilla, J., Gopinathan, C., Gopinathan, S., Ratnasamy, P.,	189161
16	A process for the preparation of syngas An improved process for the preparation of surface modified semiconducting metal oxides	Uphade, B.S., Mamman, A.S., Rajput, A.M., Choudhary, V.R.	188329
17	A process for the preparation of high silica sodium aluminosilicate	Keshavaraja, A., Ramaswamy, A.V., Vijayamohanan, K.P.,	187997

	Title	Inventor	Patent No.
1	A process for the preparation of high silica sodium aluminosilicate	Shiralkar, V.P., Eapen, M.J., Joshi, P.N., Kotasthane, A.N., Agashe, M.S.	188874
2	An improved process for the preparation of ethylene and higher olefins, using the improved supported catalyst	Uphade, B.S., Mulla, S.A.R., Choudhary, V.R.	188871
3	An improved process for the catalytic hydroformylation of alkanes	Bhanage, B.M., Divekar, S.S., Deshpande, R.M., Chaudhari, R.V.	188332
4	An improved process for the production of ethylene by non-catalytic oxidative cracking of ethane or ethane rich C2-C4 Paraffins	Rajput, A.M., Mulla, S.A.R., Choudhary, V.R.	188334
5	A process for the preparation of improved supported catalyst useful for the oxidative coupling of methane to higher hydrocarbons, oxidative conversion of natural gas to ethylene and lower olefins	Uphade, B.S., Mulla, S.A.R., Choudhary, V.R.	188538
6	An improved process for the preparation of ethylene, ethane and higher hydrocarbon	Uphade, B.S., Mulla, S.A.R., Choudhary, V.R.	188872
7	A process for the preparation of an improved polymeric device	Thomas, P.A., Turumella, P., Kulkarni, M.G.	189033
8	An improved process for the production of THPE [1,1',1",-tris (4'-hydroxyphenyl) ethane]	Sivaram, S., Ranade, V.R., Chakrapani, S., Wadgaonkar, P.P.	187237
9	An improved process for the preparation of halocumenes	Singh, A.P., Kale, S.M.	188375
10	An improved process for the preparation of (1R,cis)-(-)-caronaldehydic acid hemiacetal	Ravindranathan, T., Hiremath, S.V., Sahasrabudhe, A.B., Kulkarni, V.R., Borate, H.B.	188978
11	An improved process for the preparation of alpha-cyclodextrin glycosyltransferase enzyme	Patkar, A.Y., Gawande, B.N.	188412
12	A process for the preparation of sulphonate esters of 2,4(6)-di-O-acyl-myo-inositol-1,3,5-orthoformates	Shashidhar, M.S., Das, T.,	188417
13	A process for the preparation of an improved composition useful for promoting development of shoots from the excised embryo-axis of cotton	Agrawal, D.C., Banerjee, A.K., Kedari, P.H., Jacob, S., Hazra, S., Krishnamurthy, K.V.	189032
14	An improved process for the preparation of unsaturated hydroxy lactones	Pais, G.C.G., Pradeep Kumar, Ravindranathan, T., Rajiv Kumar	189048

Books/chapters in books

Book edited

Recent Trends in Optimisation of Chemical Engineering Systems [Proceedings of Indian National Science Academy Part A: Physical Sciences, Vol. 69, 3-4], Sp. Editors V.K.Jayaraman, B.D.Kulkarni, INSA, New Delhi.

Chapters in books

Aziridination, Renu Vyas and Bhanu M. Chanda in "Encyclopaedia of Catalysis", Wiley Interscience (USA).

Combinatorial chemistry and high throughput screening: a tool for the faster discovery of fungicides, Natu A.A. and Deshpande M.V.. Proceedings of the IV Asia Pacific Crop Protection Conference-2003. Pesticides Manufacturers & Formulators Association of India, Mumbai.

Fungal cellulases for novel industrial applications, Santosh Vyas, Anil Lachke and Absar Ahmad, in "Frontiers of Fungal Diversity in India", Eds. G.P.Rao, C.Manoharachari, D.J.Bhat, R.C.Rajak and T.N.Lakhanpal, International Book Distributing Co., Lucknow.

Gold nanoparticles formed within ordered mesoporous silica and on amorphous silica, R.Kumar, A.Ghosh, C.R.Patra, P.Mukherjee and Murali Sastry, in "Nanotechnology in Catalysis, Vol. 1", Eds. B.Zhou, S.Herman and A.Somorjai, Kluwer Academic/ Plenum Press.

Human immunodeficiency virus 1 retropepsin, B.M.Dunn and M.B.Rao, in "Handbook of Proteolytic Enzymes", Eds. A.J.Barrett, N.D.Rawlings and J.F.Woessner, Academic Press (United States of America).

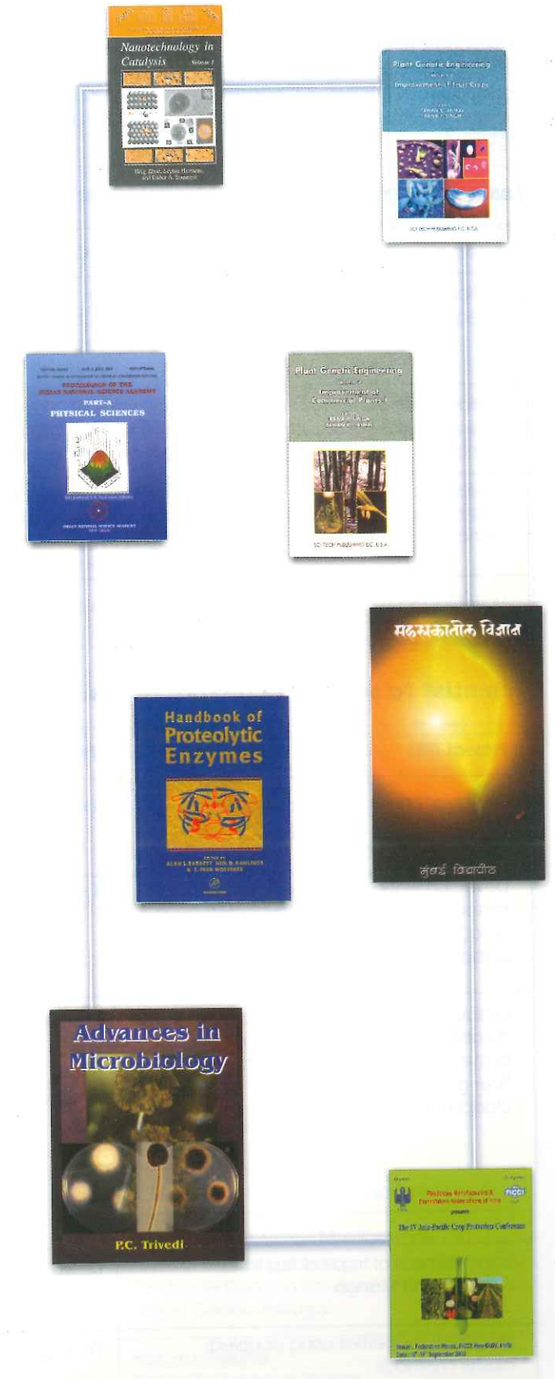
In vitro regeneration and genetic transformation of Cashewnut (Anacardium occidentale L.) in Plant Genetic Engineering vol 6, Improvement of Fruit Crops, Nadgauda Rajani and Gogte S. S. (2003), (Eds Jaiswal P. K. and Singh R. A.) Sci Tech Publishing LLC, USA.

Nanoparticle assembly through electrostatic interactions, Murali Sastry, in "Nanoparticles : Synthesis, Modification and Applications", Ed. V.Rotello, Kluwer Scientific Publishers, New York.

Nanoparticle organization at the air-water interface and in Langmuir-Blodgett films, Murali Sastry, in "Colloids and Colloid Assemblies: Synthesis, Modification, Organization and Utilization of Colloid Particles", Ed. F. Caruso, Wiley-VCH, Berlin.

Thermophilic Xylanases- Molecular and Biotechnological Perspectives, S.P.George, D.S.Nath and M.B.Rao, in "Advances in Microbiology", Ed. P.C.Trivedi, Scientific Publishers (India).

Vanaspati Jeev Tantradyan, R.S.Nadgauda, in "Sahastrakatil Vidnyan", Bombay University.



International research collaborations

NCL and its scientists have many collaborative projects with leading academic and scientific institutes and also with individual researchers. NCL as an institute has entered into Memorandum of Understandings with University of Science and Technology, Lille (USTL) and the National Institute for Applied Sciences, Lyon (INSA, Lyon), both from France, National Center for Cell Science and Vasantdada Sugar Institute, both from Pune. NCL scientists individually or as a team also have many collaborative programmes with various leading research groups from India and abroad.

Institute to institute collaborations:

External Institute	Field(s) of Collaboration	NCL Noadal Scientist (S)
National Center for Cell Science, Pune	Exploitation of biomedical potentials of fungal extracts of specific tissues relatd to hitherto unattained aspects of peptide/ protein fractionation, purification and bioactivity testing from fungi	Dr Islam Khan
National Institute for Applied Sciences, Lyon (INSA, Lyon), France	Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Mr Sanjay Nene
University of Science and Technology, Lille (USTL), France	High Field Solid State NMR Studies, Catalysis, Biochemistry, Polymer and Materials Science Engineering, Chemical and Process Engineering (Design and Development)	Dr Rajiv Kumar/ Dr S Ganapaty
Vasantdada Sugar Institute, Pune	Zeolite assisted Ethanolic Fermentation	Dr Archana Pundle

Scientist to scientist collaborations:

Project Title	NCL Partner(s)	External Partner(s)
Design of bifunctional supported non-iron catalysts for low temperature ammonia synthesis	Dr. S.B. Halligudi	Prof. V.A. Likholobov, Boreskov Institute of Catalysis Novosibirsk, Russia
Development of novel biopesticides based on fungi/ bacteria exhibiting dual antagonistic activity against plant pathogenic fungal and insect pests	Dr. M.V. Deshpande	Prof. A. Lobanok Director Institute of Microbiology, Belarus Academy of Sciences, Minsk, Belarus
Evaluation and improvement of the durability in a composite insulator: study of the degradation/stabilization of epoxy fiber glass composites coated with elastomers	Dr. R.P. Singh	Prof. J.L. Gardette Laboratoire De PhotochimieMoleculaire et Macromoleculaire (LPMM) Universite Blaise Pascal, Cedex, France Prof. J.Lacoste, ENSCCF, France Dr. Emmanuel Brocard Sediver, St.Yorre, France
Improvement of tropical fruit trees Cashew and Mango	Dr. Rajani Nadgauda	Dr Mohan Jain International Atomic Energy Agency, Vienna, Austria
Magnetic properties using coupled-cluster methods	Dr. Sourav Pal	Dr. Jozef Noga, Institute of Inorganic Chemistry Slovak Academy of Sciences Bratislava, Slovakia

Microbial Control of pest: Entomopathogenic fungi as mycoinsecticides	Dr. M.V. Deshpande	Dr. Mounir Hassani Directeur general ATLAS AGRO, Zurich, Switzerland Dr. Keller Siegfried, Swiss Federal Research Station for Agroecology and Agriculture, Zurich-Reckenholz, Switzerland
Mixing in Opaque Multiphase Systems	Dr. V.V. Ranade	Prof. M.P. Dudukovic Chemical Reaction Engineering Laboratory, Washington University at St. Louis, Washington, USA
Modeling of zeolite framework relaxation	Dr. Sourav Pal	Dr. Francois Fajula (PI) Dr. Annick Goursot (Co-PI), ENSCM, Montpellier, France
Nanoparticle assembly at the air-water interface.	Dr. Murali Sastry	Prof. D. Langevin, CNRS, Orsay, France
New thermotropic liquid crystalline polyurethanes	Dr. C. Ramesh	Prof. Anil Kumar, Department of Chemistry, IIT Bombay
Selective oxidation and aziridination of aromatic hydrocarbons by metal complexes encapsulated in micro and mesoporous solid supports	Dr. S.B. Halligudi	Prof. Stefan Ernst, University of Kaiserslautern, Kaiserslautern, Germany
Somatic hybridization of peanut (*Arachis hypogaea* L) by protoplast fusion	Dr. Sulekha Hazra	Dr. Maria-Teresa Scarano, Instituto di Genetica Vegetale - Sezione di Palermo Consiglio Nazionale delle Ricerche, Palermo, Italy
Structure and morphology of PET fibers	Dr. C. Ramesh	Dr. N. Sanjeeva Murthy, Department of Physics, University of Vermont, USA
Studies on the structure and function of metal in mesoporous materials	Dr. (Mrs) Veda Ramaswamy	Dr. Zdenek Sobalik, J. Heyrovsky Institute of Physical Chemistry, Dolejskova, Czech Republic
Study on Crystalline transition in Nylons using HTFTIR	Dr. C. Ramesh	Prof. K. Tashiro, Department of Macromolecular Science, Graduate School of Science, Osaka University, Japan
Synthesis of Functionalized Polyolefins and its Durability Improvements: Novel approach to stabilization against photochemical degradation	Dr. R.P. Singh	Dr. Maria das Merces Marques, Instituto Superior Technico, Centro de Qumica Estrutural II Lisboa Cedex, Portugal
The mechanism and kinetics of NO reduction reactions on noble surfaces from single crystal surfaces to supported model catalysts	Dr. C.S. Gopinath (PI) Ms Neelima Iyer (Co-PI)	Prof. H.J. Freund, Dept. Of Chemical Physics Frtiz-Haber Institute of Max Planck Society, Berlin, Germany

Deputations abroad

Business development

- **Dr. A.K. Lele** (USA) to meet representative & from Invista and Honeywell for discussion on project & to be undertaken at NCL, 10-18 Feb, 2004
- **Dr. M.K. Gurjar** (Germany) to attend Chemical Pharmaceutical Industrial Exhibition, 27-30 Oct, 2003
- **Dr. M.K. Gurjar** (USA) to visit various pharmaceuticals companies in USA, 30 Nov -13 Dec, 2003
- **Dr. R.V. Chaudhari** (USA) to participate as member of team for process evaluation of a process for isoporopanol by direct hydration, 10-15 Aug, 2003
- **Dr. R.V. Chaudhari** (France & UK) to visit Dupont Textiles and Interiors UK and Enki Sustainable Technologies Sainte-Foy, France for review of ongoing collaborative projects as well as a new project on hydrogenation of oligometric material, 16-29 July, 2003
- **Dr. Upendra Natarajan** (Japan) to attend special discussion sessions which include cationic Surfactant Alliance Symposium at P&G in order to discuss technical issues and finalise new business opportunities, 19-22 Jan, 2004

Bilateral /collaborative/exchange programmes

- **Dr. M.V. Badiger** (France) for carrying out research work under the IFCPAR funded project " Novel Hydrophobically Modified Polymers: Synthesis Characterisation and Rheology, 15 Feb - 14 March, 2004
- **Mr. V. Chavan** (Japan and China) to participate in the Joint International Forum on Biodiversity Information and later to participate in "Species 2000 Asia Oceania Forum", 02-16 Oct, 2003
- **Dr. M.V. Deshpande** (Switzerland, Germany and UK) INDO-SWISS collaboration in Biotechnology, 10-21 June, 2003
- **Dr. S. Ganapathy** (France) to carry out research work on the project "New Solid state NMR techniques and elucidation of the structure of molecular sieves of catalytic importance" funded by ICPAR, 01 - 30 Nov, 2003
- **Dr. K.N. Ganesh** (UK) to visit under the INSA-The Royal Society Academic Exchange Programme , 26 Aug - 07 Sep, 2003
- **Dr. S.B. Halligudi** (Russia) to work at the Institute of Catalysis Novosibirsk on the ILTP Project entitled "Design of Biofunctional supported Non-Iron Catalysts for Low-Temperature Ammonia Synthesis", 24 Aug - 08 Sept, 2003
- **Dr. S.B. Halligudi** (Germany) to visit under DST-DAAD PPP Project entitled "Selective Oxidation and Aziridination of Aromatic Hydrocarbons by Metal Complexes encapsulated in micro and mesoporous solid supports", 01-31 Oct, 2003
- **Dr. (Mrs) U.J. Mehta** (Italy) to carry out research work on the project under CSIR-CNR Programme, 15-30 Nov, 2003
- **Dr. Sourav Pal** (France) to carry out research work on the project "modelling zeolite framework relaxation" funded by IFCPAR, 12 Nov- 11 Dec, 2003
- **Dr. R.P. Singh** (France) to carry out research work under the IFCPAR funded, to visit LCOM-Chimie Des Polymer, 10 March - 16 April, 2004
- **Dr. R.P. Singh** (Portugal) to carry out research work on the project under Indo-Portugal InterGovernmental programme, 08-22 Dec, 2003
- **Dr. P.P. Wadgaonkar** (France) to carry out research work under the IFCPAR funded project "Novel Hydrophobically Modified Polymers: Synthesis Characterisation and Rheology, 15 Feb - 14 March, 2004

Conferences/ seminars/ symposia/ workshops

- **Dr. N.P. Argade** (China) to attend the International Symposium on Bioprocess and Biomolecular Engg. , 15-17 Dec, 2003
- **Mr. G.M. Chapekar** (Taiwan) to attend pre-conference school on "Advanced methods in characterisation of catalysts and Materials" , 13-18 Nov, 2003
- **Dr. R.V. Chaudhari** (Australia) to deliver keynote speech at the CHEMECA-2003 in the field of Chemical Engg. and Catalysis ; to visit RMIT to explore the possibility of establishing future collaboration between RMIT & NCL, 28 Sep - 04 Oct, 2003
- **Dr. (Mrs) V.V. Deshpande** (China) to attend the International Symposium on Bioprocess and Biomolecular Engg., 15-17 Dec, 2003
- **Dr. K.N. Ganesh** (Japan) to attend the Indo-Japan Workshop on Advanced Molecular Electronics and Bionics, 11-13 Dec, 2003
- **Dr. K.N. Ganesh** (Canada) to participate in the 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry, 10-17 Aug, 2003
- **Dr. (Mrs) V.S. Gupta** (Italy & Switzerland) to attend 10th International Wheat Genetics Symposium at Italy and attend the 8th Wheat Gluten Workshop at Italy and visit University of Zurich, Switzerland to discuss project results and research plans with the collaborators, 01-17 Sep, 2003
- **Dr. M.K. Gurjar** (Seoul, Korea) to attend KOSEF-INSA Joint Seminar on Organic synthesis under the sponsorship of INSA and KOSEF , 27-30 July, 2003
- **Dr. K. Guruswamy** (USA) to attend Gordon Research Conference on Colloidal Macromolecular and Polyelectrolyte solution, Business Development trip to discuss possibility of Indo-US project on crystallization, 01-14 Feb, 2004
- **Dr. JP Jog** (Canada) to attend the Second International Symposium on Polymer nanocomposites Science and Technology, 06-08 Oct, 2003
- **Dr. P.N. Joshi** (Taiwan) to attend pre-conference school on "Advanced methods in characterisation of catalysts and Materials" , 13-18 Nov, 2003
- **Dr. Rajiv Kumar** (Taiwan) to attend the 3rd Indo-Pacific Catalysis conference to be held jointly with 21 st Taiwan Symposium on Catalysis and Reaction Engineering (TSCRE-2003) , 16-18 Nov, 2003
- **Dr. (Mrs) V.A Kumar** (Canada) to participate in the 39th IUPAC Congress and 86th Conference of the Canadian Society for Chemistry, 10-15 Aug, 2003
- **Dr. (Mrs) S. Laxman** (China) to attend the International Symposium on Bioprocess and Biomolecular Engg. , 15-17 Dec, 2003
- **Dr. (Mrs) Mala Rao** (China) to attend the International Symposium on Bioprocess and Biomolecular Engg. , 15-17 Dec, 2003
- **Dr. (Mrs) Mayadevi S** (USA) to participate in the First Interdisciplinary Conference on Green Engineering entitled "Green Engineering: Defining the principles" , 14-22 May, 2003
- **Dr. V.V. Ranade** (Canada and USA) to present papers at 6th International conference at Vancouver, BC and institutional visits at Canada, St. Louis, USA , 17- Aug -06 Sep, 2003
- **Dr. Murali Sastry** (Australia) to attend a day's symposium on "Some Emerging Trends in Chemistry" and associated visit to carry out discussion with the staff at RMIT, 12-15 March, 2004
- **Dr. Murali Sastry** (Japan) to attend the Indo-Japan Workshop on Advanced Molecular Electronics and Bionics, 11-13 Dec, 2003
- **Dr. A.P. Singh** (Taiwan) to attend the 3rd Indo-Pacific Catalysis conference to be held jointly with 21st Taiwan Symposium on Catalysis and Reaction Engineering (TSCRE-2003) , 16-18 Nov, 2003
- **Dr. S. Sivaram** (Canada & USA) to participate in Hydrogen and Fuel Cells Conference, Vancouver, to attend two day workshop to accelerate collaboration between Canadian and Indian Counterparts, Vancouver, to attend GRA Technology Fusion Workshop on Energy, Columbus, Ohio, 8-19 June, 2003
- **Dr. S. Sivaram** (USA) to deliver an invited talk at International Union of Pure and Applied Chemistry (IUPAC, USA); International Symposium on Ionic Polymerization, Boston, to deliver an invited talk in a symposium in honour of Professor J.P. Kennedy, The University of Akron, 2-9 July, 2003
- **Dr. S. Sivaram** (Korea) to deliver an invited lecture in the International Symposium on "NT-IT-BT and Polymer" (Nano Technology Information Technology Bio Technology and Polymers) at Department of Materials Science & Engineering, KJIST, Kwangju, to deliver an invited lecture at Korea Research Institute for Chemical Technology (KRICT), Daejon 1-5, March, 2004

Fellowships

- **Dr. D.C. Agrawal** (Germany) to avail resumption of Alexander Von Humboldt Fellowship, 15 Sep - 15 Dec, 2003
- **Dr. V. R. Choudhary** (Japan) to avail JSPS Fellowship to conduct research under the leadership of Prof. M. Ichikawa, Kokkaida University, 31 July - 28 Sep, 2003
- **Dr M. Karthikeyan** (USA) to avail BOYCAST fellowship to conduct research under the guidance of Prof Alex Tropsha, School of Pharmacy, University of North Carolina at Chapel Hill, March 2003- March 2004
- **Dr. Pradeep Kumar** (Germany) to avail resumption of Alexander Von Humboldt Fellowship, 01 - 31 Dec, 2003
- **Dr. S.A.R. Mulla** (Japan) to avail Post-Doctoral Fellowship for Foreign Researchers, Two years from 01 Nov 2003
- **Dr. Paul Ratnasamy** (Germany) to avail the Alexander Von Humboldt Fellowship at the University of Munich, 01 Sep - 30 Nov, 2003

Meetings

- **Dr. N.P. Argade** (Italy) to attend Expert Group Meeting (EGM) on "Combinational Chemistry, Molecular Design and Promotion of Related Projects", 03-4 July, 2003
- **Mr V.S. Chavan** (USA) to attend the meeting of the ocean Biogeographic Information system, International Committee and Regional Nodes Meeting, 12 March - 8 April, 2004
- **Mr V. Chavan** (Bangladesh) to participate in the meeting of Global Biodiversity Forum - South Asia, 15-19 June, 2003
- **Dr. S. Devotta** (Canada) to participate in the 23rd Meeting of the Open Ended working group of the parties to the Montreal Protocol on an invitation from UNEP to represent TFDT/TEAP, 07-11 July, 2003
- **Dr. V.R. Pedireddi** (Singapore) to attend the ICMAT 2003, 07 - 12 Dec, 2003
- **Dr. S. Sivaram** (Germany) nominated by DGCSIR as a member of the four-member Indian delegation to CSIR FzJ Cooperative Science Programme, International Bureau of the German Ministry of Education and Research (BMBF), 14-20 September, 2003
- **Dr. S. Sivaram** (Germany) to represent DGCSIR in the 3rd Annual Meeting of the Global Research Alliance Principals, Nerve Centre, Bonn, 25-29 January, 2004

EOL/ sabbatical leave

- **Dr. S.K. Chaudhari** (Spain) to visit Department of D'Entinginyeria Marcanica, Universitat Rovira I Virgili, Tarragona Spain, one year from 01 Aug 2003
- **Dr. S.D. Deshpande** (South Korea) for Post Doctoral Fellowship in the Creative Research Centre for EAPap Actuator, Inha University, South Korea., ten months from 13 Aug 2003
- **Dr. A.P. Giri** (USA) to carry out specific work at Washington State University sponsored by Mcknight Foundation, USA, 01 Sep-30 Nov, 2003
- **Dr. I.S. Mulla** (South Korea) as International fellow at Chemical technology Division of Korea Research Institute of Chemical Technology, one year form 16 Jan 2004
- **Mr M. Muthukrishnan** (Japan) for Post Doctoral Fellowship at Kyushu Institute of Technology, Kyushu, Japan under Prof. Norikazu Nishino, one year from 01 Oct 2003

Student participation in conference/ research projects

- **Mr. D.M.R.S. Reddy** (Switzerland) to visit University of Zurich under the Indo-Swiss collaboration in biotechnology, Aug-Nov. 2003
- **Ms. D.P. Sawant** (Germany) to visit University of Kaiserslauten under Indo-German DST-DAAD Project, Oct.- Dec. 2003
- **Mr. Ajay Srinivasan** (UK) to visit University of Durham under the McKnight Foundation, May - Dec. 2003
- **Ms. Manasi Telang** (USA) to visit Washington State University, Pullman under the McKnight Foundation, Aug.-2003 - April 2004
- **Ms. Trupti M. Maddanimath** (USA) Rensselaer Polytechnic Institute, New York as visiting scholar, April 2003 - March 2004
- **Mr. Niranjan Ramgir** (Canada) to attend the second IEE international conference on sensors, Toronto, Oct 22-24, 2003

Lectures /seminars delivered by visitors

Speaker	Title (S)
Dr. Jürg Enkerli Agroscope FAL-Reckenholz, Zurich, Switzerland	Validation of biological pest control strategies: Microsatellite markers as a powerful tool
Dr. Klaus Weishaupt Managing Director, WITec Germany	Confocal Raman microscope as a tool of research in physical, chemical and Life science applications
Dr. Krishnanand Chattopadhyay Washington University, School of Medicine, St. Louis, USA	Protein folding and fluorescence correlation spectroscopy: Studies with intestinal fatty acid binding protein
Dr. Lubos Horny Centre for Computational Chemistry,, University of Georgia, USA	Brillouin-Wigner approach multi-reference coupled-cluster theories
Dr. Lynne B. McCusker ETH, Zurich, Switzerland	Solving zeolite framework structures with FOCUS
Dr. M. Eswaramoorthy National Institute of Advanced Industrial Science and Technology, Tsukuba, Japan	Organoclays with organized structures- A modern morphology?
Dr. Martin Hartmann Universitat Kaiserslautern, Germany	Mesoporous molecular sieves in separation and catalysis - Concepts and perspectives
Dr. N. Dastagiri Reddy Univ. of Calgary, Alberta, Canada	Synthesis of some Dirhenium complexes, aluminum nitrogen clusters and catalysts for copolymerization of polar and non polar monomers
Dr. Nilashis Nandi Birla Institute of Technology and Science. Pilani, Rajasthan	Theoretical study of complex chemical and biomimetic systems
Dr. P. C. Ghosh Institute for Materials and Process in Energy System (IWV-3), Julich, Germany	Measurement of current density distribution in fuel cell
Dr. P. K. Madhu Tata Institute of Fundamental Research, Mumbai	Spinning rotors and rotating spins in the NMR of solid-state
Dr. Pankaj Poddar Department of Physics, University of South Florida, Tampa, USA	Transport. magnetic and magnetocaloric properties of arrays of nanoparticles
Dr. Parasu Veera University of Twente, The Netherlands	Hydrogen response of industrial metallocene catalyst for the production of polypropylene
Dr. Prasanna V. Joshi Senior Scientist, ExxonMobil Process Research	Compositional based models for refinery processes
Dr. Pratibha Srivastava National Cancer Institute, Bethesda, USA	Expedient syntheses of arenes and heteroarenes leading to potentially useful pharmacophore
Dr. R. P. Iyer Vice President and Chief Scientific Officer, Spring Bank Technologies, Inc. MA, USA	Design, synthesis and application of reagents for gene synthesis on solid support
Dr. Robert Jones Jr. Basell Polyolefine GmbH, Ludwigshafen, Germany 67056	New catalysts for polyolefins

Speaker	Title (S)
Dr. Sachin Borkar Technical University of Denmark, Lyngby, Denmark	Synthesis and characterization of functional Di-block copolymers
Dr. Sailesh Kumar UOP Des Plaines, USA	Modeling of multiphase systems
Dr. Sanjoy Mullick Philips Electronics, Singapore	Selected research projects presentation
Dr. Sapna Ravindranathan Ecole Polytechnique Ferderale, 1015 Lausanne, Switzerland	Cross-correlated relaxation in biomolecular systems
Dr. Simoni Arizzi Technical Director for Nylon and Spandex (Lycra) InVista, USA	Future R&D directions at InVista
Dr. Suneel Kunamaneni Dept of Physics & Astronomy, University of Leeds, UK	Rheology of hyperbranched polymers
Dr. Swapan K. Ghosh Chemistry Division, BARC, Mumbai	Concept of density in chemistry and materials modeling
Dr. T.G. Ajithkumar Department of Physical Chemistry, University of Nijmegen, The Netherlands	Homonuclear correlation experiments of Half-Integer
Dr. T. Rajgopal Hindustan Lever Research Centre, Mumbai	Occupational health. safety & environment in a chemical laboratory
Dr. V. Thangadurai University of Kiel, Germany	Materials aspects of solid state ionic devices
Dr. Vaishali Shah Carnegie Mellon University, Pittsburgh, USA	Modeling of materials
Dr. Venkatesan V. Krishnan Department of Chemical Engineering, University of Pennsylvania, Philadelphia, USA	Development of novel copper-ceria (CeO_2) Anodes for direct hydrocarbon conversion solid oxide fuel cells (SOFC's)
Dr. Y.R. Mahajan Defence Metallurgical Research Laboratory, Hyderabad	Nature inspired innovation: Ceramic honeycomb structure and its technological potential
Mr. Alberto Araoz Former UNIDO Deputy Director-General for Technology and Foreign Investment	Using science for development: some current ideas
Ms. Payel Das Rice University, USA	A Combined approach of theory and experiment to characterize protein folding
Prof. A.K. Shukla Central Electrochemical Research Institute, Karaikudi	Mixed-reactants direct methanol fuel cells
Prof. Andrea Vasella ETH, Zurich, Switzerland	1. Glycosidase Inhibitors and the mechanism of Action of glycosidase enzymes 2. Towards new oligonucleotide analogues
Prof. D. K. Chattoraj Jadavpur University, Kolkata	Interaction of water vapour with biocolloids and some monolayer properties of model biosurfaces

Speaker	Title (S)
Prof. Frederick J. Krambeck Johns Hopkins University, Whiting School of Engineering, USA	Glycosylation reaction kinetics
Prof. G. Ramanath RPI, Troy, NY, USA	Cool nano structures: Directed assembly and new applications
Prof. Gautam Desiraju School of Chemistry, Central University, Hyderabad.	The hydrogen bridge: Interaction without borders
Prof. Goverdhan Mehta Director, Indian Institute of Science, Bangalore	Design of new molecular objects : Art and logic in organic synthesis
Prof. J. Gopalakrishnan Indian Institute of Science, Bangalore	Turning solids into materials : Chemistry plays a key role
Prof. Jacques Mortier Universite du Maine, Le Mans, France	The carboxylic acid as an effective director of ortholithiation
Prof. K. V. Rao Department of Materials Science, Royal Institute of Technology, Sweden	Above room temperature ferromagnetism in Mn doped ZnO
Prof. Kenneth J. Klabunde Department of Chemistry, Kansas State University, Manhattan, USA	Nanomaterials for environmental remediation: Protection from toxic chemicals and weapons of mass destruction
Prof. L.M. Harwood School of Chemistry, Whiteknights, Reading, RG6 6AD, UK	Ultra-high pressure as a mild synthetic tool: The IMDAF approach to phorbol
Prof. Ludmila Audouin Institute of Engineering Technology, Paris, France	Ageing of polyethylene cables used in nuclear environment
Prof. M. Anpo Osaka Prefecture University, Osaka, Japan	New trends in the science and technology in TiO2 photocatalysis
Prof. M. Ghafari Institute of materials science, Darmstadt University of Technology, Germany	Magnetism of iron nanoparticles
Prof. M.P. Dudukovic Director, Washington University at St. Louis, Missouri 63130, USA	Advances in multiphase reaction engineering
Prof. M.S. Swaminathan Swaminathan Research Foundation, Chennai	Science and sustained agriculture
Prof. Mahendra K. Sunkara University of Louisville, USA	Bulk synthesis strategies for Inorganic nanowires, nanotubes and nanowire Networks
Prof. Mangala Sunder Krishnan IIT, Chennai	Quantum teleportation : A statistical model for EPR correlation
Prof. Moti Lal University of Liverpool, UK	Molecular simulation dynamics of the solvation processes of nanoparticles in supercritical fluids
Prof. Patrick Metzner ENSICAEN University, France	Chiral sulfoxides as efficient tools for the stereocontrol of [3,3] sigmatropic rearrangements

Speaker	Title (S)
Dr. Amish Joshi National Physical Laboratory, New Delhi	Structure and superconductivity of R123 [R = Ho, Dy] and binary 1:2 compound
Dr. Anand Bachhawat Institute of Microbial Technology, Chandigarh	Glutathione transporters, drugs, and drug resistance: tapping the power of yeast genetics
Dr. Anant Patel Federal Agricultural Research Centre, Braunschweig, Germany	Formulation of biocontrol agents
Dr. Anthony D. William University of Geneva, Switzerland	Organophosphorus compounds-versatile substrates in transition metal-catalyzed cross-coupling reactions and natural product synthesis
Dr. Anuradha Moulee Trainee Attorney, Baldwin Shelston Waters, Australia	Validity and interpretation of patent specifications
Dr. Atul D. Dhale Michigan State University, East Lansing MI, USA	Recovery of glycols from aqueous solution via reactive distillation
Dr. Atul Deshmane Chief Engineer, eTransIT Solutions Inc., Bellingham, USA	Fuel cell applications engineering for cell phone
Dr. Ayusman Sen Department of Chemistry, The Pennsylvania State Univ., USA	Polymer synthesis: From macro to nano
Dr. Chandrashekhar Verma University of York, UK	Computer simulation in modern molecular biology
Dr. Christophe Chassenieux ESPCI, Paris, France	Shear Induced gellification in amphiphilic polymers
Dr. D. Ajitha Department of Chemistry, University of Lund, Sweden	Photodissociation dynamics of alkyl halides
Dr. Fabrice Odobel Laboratoire de synthese organique, Cedex 3, France	Electronically coupled porphyrin systems
Dr. George Frater Director, Research Centre, Givaudan, Switzerland	Fragrant molecules related research chemistry
Dr. Gopinathan Sankar Royal Institution of Great Britain, U.K.	1. Spectroscopic characterization of heterogeneous catalysis: Fundamentals of X- rays 2. Spectroscopic characterization of heterogeneous catalysis: X-ray diffraction and Scattering Techniques 3. X-ray absorption and X-ray photoelectron spectroscopy for catalytic materials 4. Spectroscopic characterization of heterogeneous catalysis: X-ray absorption Spectroscopy
Dr. Jean Jenck Rhodia, France	Integrated multi-scale process design for sustainable chemical technologies
Dr. Jeevanandam Pethaiyan Department of Chemistry, Kansas State University, Manhattan, USA	Surfactant coated magnesium oxide nanoparticles: Properties and applications

Speaker	Title (S)
Dr. Jeff Kenvin Scientist, Micromeritics Instruments Corpn., USA	Catalysis, characterization using sorption and temperature programmed techniques
Prof. Philip Cohen Royal Society Research Professor, University of Dundee, UK	Kinase Inhibitors : Drugs for 21st Century
Prof. Pramod Kale Former Director. VSSC. ISRO	Water
Prof. Pushan Ayyub TIFR, Homi Bhabha Road, Mumbai	Understanding the size dependence of physical properties
Prof. R. Dhamodharan IIT, Chennai	Surface-Initiated living polymerizations under mild conditions
Prof. R. Ramaswamy Jawaharlal Nehru University, New Delhi	The dynamics and structures of finite atomic clusters
Prof. Rajendra Prasad Jawaharlal Nehru University, New Delhi	Multidrug resistance : an emerging threat
Prof. S. Ramakrishnan Indian Institute of Science, Bangalore	Melt transetherification polycondensation - A novel route to polyethers
Prof. Simeon Arseniyadis Centre National De La Recherche Scientifique, Gif Sur Yvette Cedea- France	Serendipity and target driven methodologies: Synthetic strategies towards selected targets
Prof. Sudipta Seal, University of Central Florida, Orlando, USA	Role of organics in nanomaterial synthesis and
Prof. Suresh C. Mehrotra Dr. Babasaheb Ambedkar Marathwada University, Aurangabad	Microwave induced polarisation in polar liquids and their mixtures
Prof. Thomas Wirth Cardiff University, U. K.	New chiral electrophiles: Challenges from selenium and Iodine
Prof. Vasundhara Singh Thapar School of Engineering and Technology	Heterogeneously catalyzed reactions using US and MW
Prof. W. Hoelderich Dept of Chemical Technology & Heterogeneous Catalysis, RWTH Aachen, Germany	1. Fine chemical transformation using heterogeneous catalysis: on the examples of fragrances and flavours 2. Development of a new caprolactam-process: catalyst design and process engineering 3. Immobilization of chiral homogeneous catalysts and their use for oxidation and hydrogenation reactions 4. Oxidation reactions in the synthesis of intermediate chemicals using Environmentally benign oxidants and the right reactor system 5. New heterogeneously catalyzed processes for environmentally benign and sustainable chemical production
Prof. Y. Gnanou Univ. of Bordeaux, France	Polymer-based supramolecular structures for nanoscale applications
Dr. M.K. Bhat, Scientist, Institute of Food Research, Norwich Research Park, Norwich, UK	Plant cell wall degrading esnzymes

Invited talks / lectures delivered by NCL scientists

Mr. Vishwas Chavan

- Biodiversity Informatics: A Quite Revolution, International Workshop on Bioinformatics at Karpagam Arts & Science College, Coimbatore, March 18-20, 2004.

Dr. M.V. Deshpande

- Chitin metabolising enzymes as a target for fungicides, Brain storming session of CSIR NMITLI programme, Bangalore, April 2003.
- Novel approaches for the control of plant pathogenic fungi and insects in agriculture: entomopathogenic fungi as mycoinsecticides, Institute of Biological control, Darmstadt, Germany, June 2003.
- Dimorphism in fungi, Cardiff University, Cardiff, UK, June 2003.
- Biochemical and molecular aspects of fungal cell wall synthesis and dimorphic transition in *Benjaminiella poitrasii*. ISMPP, Jaipur, October 2003.
- Biopesticides: a viable alternative for the management of pests, NMU, Jalgaon, November 2003.

Dr. K.N. Ganesh

- DNA - Amine interactions: From dendrimers to monolayers and nanoparticles, at IUPAC meeting on Chemistry, Ottawa, Canada, August 13, 2003.
- Conformationally Constrained PNA Analogues: Design, Synthesis and Biological Evaluation, at Department of Chemistry, University of Sheffield, UK, August 29, 2003.
- Direct binding of HIV-1 Tat to NFêB enhancer sequence: Role in viral and cellular gene expression, at Krebs Institute of Molecular Biology, University of Sheffield, UK August 30, 2003.
- DNA - Amine interactions: From dendrimers to monolayers and nanoparticles at 5th Cambridge Symposium on Chemistry and Biology of Nucleic Acids, Queen's College, Cambridge, September 3, 2003.
- Conformationally Constrained PNA Analogues: Design, Synthesis and Biological Evaluation, Royal Society Discussion meeting on bioorganic chemistry, September 5, 2003.
- Collagen Structure and the tale of two prolines: 4-Aminoproline Collagen, at Department of Chemistry and biomolecular crystallography, University of York, UK, September 7, 2003.
- Designed DNA and PNA analogues as building blocks for functional nanoparticles Indo-Japan workshop on Advanced Molecular Electronics and Bionics, held at SELEX as a powerful tool to explore DNA-protein interactions: Application to HIV tat interactions, International Conference on Emerging Frontiers at the Interface of Chemistry and Biology, Regional Research Laboratory, Trivandrum, April 28-30, 2003.
- DNA as a template receptor for organizing cationic ligands: From monolayers to Nanoparticles & The tale of two pralines and collagen structure: 4 Aminoproline collagen, Department of Chemistry, IIT, Madras July 7, 2003.
- Conformationally constrained pyrroliodine PNA analogs Lecture at Aurigene, Bangalore, July 9, 2003.
- Genomics and Drug development, ICMR workshop on Human Genetics for Students, LTM Medical College, Sion, Mumbai, July 12, 2003.
- DNA - Gold Composite Nanoparticles: Fabrication and Potential Applications in Diagnostics, Nanotechnology workshop, Delhi University, October 11, 2004.
- DNA structure based drug design: (1) DNA structure and Interactions with drugs and proteins and (2) DNA analogues and Antisense Chemotherapeutics Workshop for College Teachers, JNCASR Bangalore and FCBS, Trivandrum, Kottayam, November 17-18, 2003.
- 4-Aminoproline collagen: Synthesis and triplex stabilities Lecture at Aurigene, Bangalore, November, 20, 2003.
- Novel PNA analogues: Towards DNA/RNA hybridization selectivity, Emerging Directions in Chemical Sciences: JNCASR, Bangalore, November 26, 2003.

Dr. (Mrs) Vidya Gupta

- Plant proteinase inhibitors and amylase inhibitors to combat insect attack on crop plants, Brain storming session on Bioprospecting of genes, enzymes and molecules at Department of Biotechnology, New Delhi, June 12, 2003.
- Molecular markers for conservation of biodiversity, Refresher's course on medicinal plants, their conservation and utilization at Botany Department, University of Pune, November 17, 2003.
- Molecular markers: A concept, Series of Lectures in Biotechnology and Bioinformatics organized at Bioinformatics Centre, University of Pune, December 10, 2003.
- Non-host plant proteinase inhibitors for acquiring insect resistance in host plants, Lead lecture at XXVII All India Cell Biology Conference and International Symposium-Frontiers in Biomedical Research and Technologies at University of Pune, January 9, 2004
- Increasing efficiency of chickpea productivity, Invited lecture at University of Agricultural Sciences, Dharwad, February 17, 2004.

- Potential of molecular marker technology in wheat improvement invited lecture at Punjab Agricultural University, Ludhiana during workshop on integrating molecular markers technology with wheat improvement, March 13, 2004.

Dr. M.K. Gurjar

- Can Chiral Drug Development Improve Indian Pharmaceuticals Performance at IDMA- TTA Seminar on "Role of Technology to meet WTO Challenges", Mumbai, August 30, 2003.
- Chiral Drug and its benefits in Seminar on Emerging Trends in Organic Synthesis at MS University Baroda, October 12, 2003.
- Emerging Trends in Chemical Sciences in New Millenium at Symposium on, Shivaji College, Amravati, February 5-6, 2004.

Dr. (Mrs) S.P. Joshi

- Methods in Extraction, Isolation, Separation and Identification at UGC sponsored Refresher Course in Life Sciences for teachers in College and University Departments with the theme :Medicinal Plants their Conservation and Utilization; at Botany Department, Pune University, November 11, 2003.

Dr. P.A. Joy

- Two lectures on Recent Trends in Applied Physics, at the ISTE-AICTE Short Term National Level Training Programme at Vishwakarma Institute of Technology, Pune, for engineering college teachers, May 2003.
- Current trends in magnetic materials, in the national symposium on current trends in chemical research, Guwahati University, February 27-28, 2004.

Dr. S. Krishnan

- Biodiversity Informatics: Challenges and Potential at the regional head's meet, Zoological Survey of India, Pune, December 2003.

Dr. B.D. Kulkarni

- Chemical engineering education and research: new challenges HL Roy Memorial lecture, at IIChE annual congress in Bhubaneswar, December 19, 2003.
- Process intensification strategies R Tripathi Memorial lecture at Chem Engg Dept at Banaras Hindu University, August 8, 2003.
- Global challenge in Chemical engineering PS Murthy Memorial lecture at IICT, Hyderabad, January 10, 2004.

Dr. (Mrs) R.S. Nadgauda

- Tissue Culture of Medicinal Plants, at Sinhagad College of Pharmacy, Pune, November 13, 2003.
- Tissue Culture Techniques, in a programme"Face to Face with Scientists" organised by Maharashtra Academy of Sciences and Bal Vidnyan Chalwal, Pune, December 6, 2003.

Dr. A.A. Natu

- Applications of GC MS, S.D. R & D center Tarapur, Mumbai, August, 2003.
- Fundamentals of Combinatorial chemistry, Ruia College, Mumbai, September, 2003.
- Application of hyphenated techniques Ananalysis HEMRL, Pune September, 2003.
- High through put screening and natural product processing, IHBT, Palampur, September, 2003.
- Combinatorial Chemistry present and future perspectives, Reliance Life sciences, Mumbai, September, 2003.
- Leadership in Pharma R&D. CDRI, Lucknow, December, 2003.

Mrs. V. A. Parasharami

- Plant Tissue Culture Techniques in a programme "Face to Face with Scientists" organized by Maharashtra Academy of Sciences, at Dnyan Prabodhini, Pune, December 13, 2003.

Dr. V.R. Pedireddi

- The Hydrogen Bond: Wonders and Miracles in Chemistry and Biology, RSC-West India Section- Young Scientist Coloquium: Mumbai, October, 30, 2003.

Dr. Pradeep Kumar

- Enantioselective synthesis of bioactive molecules at institute of organic Chemistry, University of Tuebingen, Germany, November 4, 2003.

Dr. Rajiv Kumar

- The "Prof. Rajadhyaksha lecture" at University Institute of Chemical Technology, Mumbai, August 22, 2003.

Dr. C.V. Rode

- Two lectures on Nanoparticles in catalysis: Activity enhancement and selectivity tuning and Supercritical carbon dioxide: Alternative medium for sustainable technologies at Ruia College, Mumbai, October, 2003.

Dr. S. Sivaram

- Building Industry R&D Relationships: Perspectives from NCL, BASF R&D Silver Jubilee Celebration, Mumbai, April 9, 2003.
- Towards a Sustainable World of Materials : Learning from Nature, Invited Lecture, Technology Day Function, M/s. Pidilite Industries Ltd., Mumbai, May 12, 2003.
- Terminal Hydroxyl Functionalized Poly(Methyl Methacrylate)s By Living Anionic Polymerization : Synthesis And Applications, Invited Lecture in International Symposium "Ionic Polymerization '03", Boston, USA, July 3, 2003.
- Self Assembly in Macromolecular Systems: Functional Polymers and Polymer Surfaces, Invited Lecture, International Symposium, "Visions in Macromolecular Engineering: The Akron Legacy", University of Akron, USA, July 7, 2003.

- The Impact of Nanotechnology in Macromolecules: Approach to Novel Functional Materials, Professor N.R. Kamath Memorial Lecture, University of Mumbai, September 8, 2003.
- Chemical Sciences Group of Laboratories in CSIR: An Overview, Julich, Germany, September 16, 2003.
- Chemical Sciences Group of Laboratories in CSIR : An Overview, Berlin, Germany, September 19, 2003.
- Polymer Chemistry for the Design Of New Materials, Invited Speaker, International Symposium on "Emerging Directions in Chemical Sciences", IISc., Bangalore, November 26, 2003.
- Novel Metals And Ligands, Indo-US Conference on Recent Advances in Organo-metallic Catalysis and Olefin Polymerization, Chennai, December 12, 2003.
- Preparation of Polymer-Layered Silicate (PLS) Nanocomposites by *in-situ* intercalative polymerization, Asian Paints Padma Bhushan Dr. R.A. Mashelkar Medal and Distinguished Speakership Award Endowment for Innovators and Science Leaders, IIChE, Bhubaneshwar, December 20, 2003.
- Chemical Sciences: Opportunities and Strategies, Lecture delivered at CSIR Annual Business Meet 2004, NCL, Pune, February 20, 2004.
- Towards A Sustainable World of Materials: Learning From Nature, Science Day Lecture delivered at High Energy Materials Research Laboratory, Pune, February 28, 2004.
- Terminal Hydroxyl Functional Poly(methyl methacrylate)s by Living Anionic Polymerization : Synthesis and Applications, Invited Lecture in the International Symposium on "NT-IT-BT and Polymer" (Nano Technology Information Technology Bio Technology and Polymers), Department of Materials Science & Engineering, KJIST, Kwangju, Korea, March 3-4, 2004.

Dr. S. Sivasanker

A plenary lecture at National Environmental Engineering Research Institute, Nagpur, August 22, 2003.

Dr. C.G. Suresh

The catalytic diad, self-proteolysis and other features of a structural superfamily of proteins called – terminal nucleophile hydrolases in "National Symposium on Emerging Trends in Bioinformatics" held at University of Pune, December 18, 2003

Dr. A.J. Varma

Green Polymers for Future Generations organized by All-India Plastic Manufacturers Association and MIT Pune, March 4, 2004

Conferences / seminars / workshops organised

30-04-2003: Symposium on "Advances in Polymer Science" in honour of Dr. S.P. Vernekar, Head, Polymer Chemistry Division on the eve of his superannuatio

30-05-2003: Symposium on "Catalysis Research in India: some highlights" in honour of Dr A.V. Ramaswamy, Head, Inorganic & Catalysis Division on the eve of his superannuation

18 & 19-07-2003: Combinatorial Techniques in Drug Discovery

19 & 20-09-2003: Royal Society of Chemistry Students Symposium

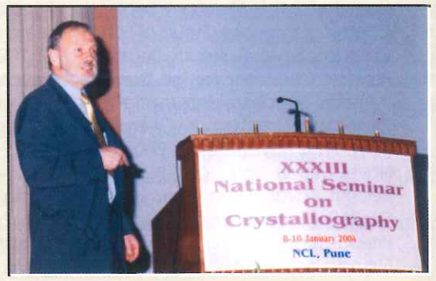
3-11-2003: POST NOST International Symposium in Organic on "Recent Developments in Organic Chemistry"

8-10 Jan 2004: XXXIII National Seminar on Crystallography

19-22 Jan, 2004: Science & Engineering Research Council School at NCL

2 & 3 Feb 2004: Workshop on Organic Synthesis Directed towards Chemical Biology & Chemical Genetics

15-3-2004: InnoCentive Annual Conference on "Innovation in Chemical & Biological Sciences"



Major awards

CSIR Technology award (2003)

Dr P.P. Wadgaonkar receiving the award on behalf of the team

A process for manufacture of 1,1',1"-Tris(4'-hydroxyphenyl) ethane (THPE) developed by Polymer Chemistry and Process Development Divisions of National Chemical Laboratory, Pune bagged the CSIR Technology Award. The project team includes: Dr. S. Sivaram, Dr. C.V. Avadhani, Dr. S. Chakrapani, and Dr. P.P. Wadgaonkar from Polymer Chemistry Division and Dr. S. Devotta, Dr. V.R. Ranade, Dr. G.R. Venkitakrishnan, Mr. S. Gopichand, Mr. H.G. Jogelkar, Mr. A.R. Joshi, Mr. R.S. Karnik, Mr. V.G. Kulkarni, Mr. Nandkishore, Mr. A. V. Palghadmal, Dr. M.G. Parande, Dr. M.S. Qureshi, Mr. M.B. Unde and Dr. J.G. Wadkar from Process Development Division.

CSIR Young scientist award (2003)

Dr. CV Ramana of Organic Chemistry (Technology) Division of National Chemical Laboratory, Pune received the **CSIR Young Scientist Award in Chemical Sciences** for his work on "The studies of the synthesis of natural products important to medicine and synthesis of designer molecules".

Dr. Upendra Natarajan of Polymer Chemistry Division of National Chemical Laboratory, Pune received the **CSIR Young Scientist Award in Engineering Sciences** for his work on "Molecular simulation and modeling studies to understand the conformational properties and chemical structure-property relationships in industrially relevant synthetic polymers".

Other awards/ recognitions

Vishwakarma Medal (INSA) Vice-President of the Indian National Science Academy Chemcon Distinguished Speaker Asian Paints Dr. R.A. Mashelkar Medal and Distinguished Speakership Award for Innovators and Science Leaders, IIChE	Dr. S. Sivaram
Srinivasa Ramanujan Research Professorship by the Indian National Science Academy	Dr. Paul Ratnasamy
CSIR Bronze Medal	Dr. K. Vijayamohanan
Organisation of Pharmaceutical Producers of India (OPPI) Scientist Award	Dr. S.P. Chavan
Plastic Udyog Ratna Award	Dr. R.P. Singh
INSA Medal for Prof. T.R. Seshadri 70th Birth Anniversary Commemoration Meda	Dr. Ganesh Pandey
Vasantrao Naik Social Forestry Award	Dr. (Mrs) Rajani Nadgauda
Associate Member of IUPAC Division of Organic and Biomolecular Chemistry	Dr. K.N. Ganesh
IUPAC National Committee	Dr. Murali Sastry

Members of board of directors of industries

Dr S Sivaram
- Asian Paints Ltd., Mumbai
- GMM Pfaudler Ltd., Mumbai

Dr Paul Ratnasamy
- Hindustan Organic Chemicals Ltd., Mumbai

Dr MK Gurjar
- Emcure Pharmaceuticals, Pune
- Cipla, Mumbai

Dr RV Chaudhari
- Bilcare Ltd, Pune

Dr AA Natu
- Tonira Pharma, Vadodara

Dr. (Mrs.) R.D. Wakharkar
- Bakul Finechem Research Centre, Mumbai

Editor/ editorial board members of journals

Dr. Anil Kumar
- Indian Journal of Chemistry Section A, NISCAIR (CSIR), New Delhi
- Editor (Chemistry), Proceedings of The National Academy of Sciences (India), Allahabad

Dr. M.V. Deshpande
- Indian Journal of Mycology and Plant Pathology, Indian Society of Mycology and Plant Pathology, Udaipur

Dr. K.N. Ganesh
- Indian Journal of Chemistry Section B, NISCAIR (CSIR), New Delhi

Dr. (Mrs) Vidya Gupta
- Plant Cell Biotechnology & Molecular Biology, Society for Biology and Biotechnology, Salem

Dr. M.K. Gurjar
- Associate Editor, Synthetic Communications, Marcel Dekker, USA
- Carbohydrate Letters, Harwood Academic Publishers, Paris, France
- Organic Process Research & Development, American Chemical Society, USA

Dr. B.D. Kulkarni
- Chemical Engineering Science, Pergamon/ Elsevier, UK
- Industrial and Engineering Chemical Research, American Chemical Society, USA

Dr. (Mrs) Rajani Nadgauda
- Plant Cell Biotechnology & Molecular Biology, Society for Biology and Biotechnology, Salem
- Physiology & Molecular Biology of Plants, Lucknow

Dr. S. Pal
- Board of Advisors, Springboard, Inc. (Engineering education), USA
- International Journal of Molecular Sciences, MDP International, Switzerland
- Journal of Chemical Sciences, The Indian Academy of Sciences, Bangalore

Dr. Rajiv Kumar
- Applied Catalysis A: General, Elsevier, The Netherlands
  Bulletin of Catalysis Society of India, Chennai

Dr. Paul Ratnasamy
- Applied Catalysis, Elsevier, The Netherlands
- Catalysis letters, Kluwer, USA
- Catalysis Surveys from Asia, Kluwer, USA
- CATTECH, Kluwer/ Plenum, USA
- Journal of Catalysis, Elsevier, The Netherlands
- Microporous and Mesoporous Materials, Elsevier, The Netherlands
- Topics in Catalysis, Kluwer, USA

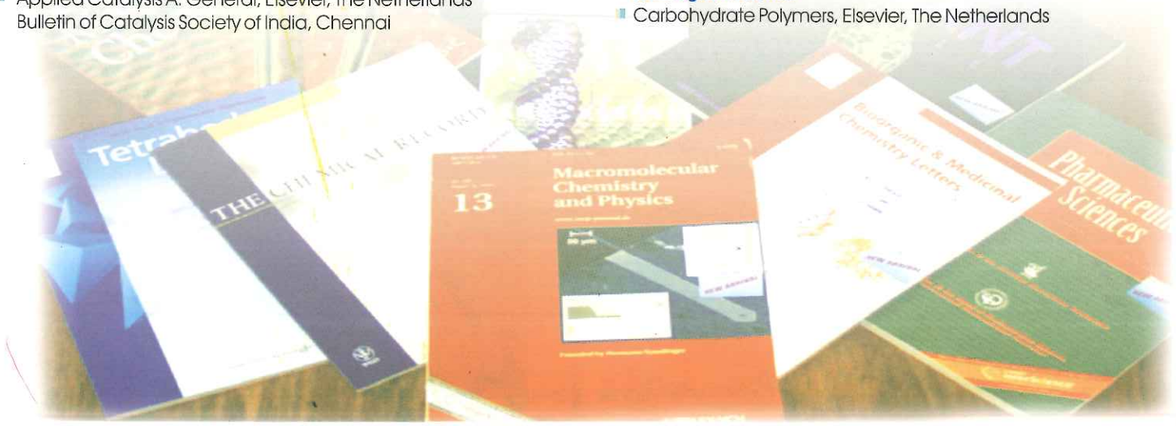
Dr. Murali Sastry
- Associate Editor (Asia), Applied Nanoscience, Open Mind Journals, Auckland, New Zealand
- Journal of Biomedical Nanotechnology, American Scientific Publishers, USA
- Journal of Colloid and Interface Science, Elsevier, The Netherlands

Dr. S. Sivaram
- Bulletin of Materials Science, The Indian Academy of Sciences, Bangalore
- Designed Monomers and Polymers, VSP International Science Publishers, The Netherlands
- Indian Journal of Chemical Technology, NISCAIR (CSIR), New Delhi
- Journal of Scientific and Industrial Research, NISCAIR (CSIR), New Delhi
- International Journal of Polymeric Materials, Gordon and Breach Publishers, New York, USA
- Journal of Polymer Materials, Oxford and IBH Publishers, New Delhi
- Journal of Chemical Sciences, The Indian Academy of Sciences, Bangalore
- Regional Editor for India, Polymer International, Society of Chemical Industry, UK

Dr S. Sivasanker
- Catalysis Surveys from Asia, Kluwer, USA

Dr. (Mrs) V.S. Tare
- Journal of Environmental Biology, Triveni Publishers, Lucknow

Dr. Anjani Varma
- Carbohydrate Polymers, Elsevier, The Netherlands



NCL research foundation

The National Chemical Laboratory Research Foundation (NCL RF), a non-profit organization was established in 1991 with a mission to promote excellence in science and technology and build an environment in which everyone in NCL strives to improve their scientific, technical and R&D support skills and reach higher goals in R&D activity. It aims at bringing creative research, knowledgebase and innovative technologies into clear focus that NCL considers important for the furtherance of the goals in science and technology.

NCL-RF has the primary aim to motivate and recognize the high level of team and individual efforts of scientists, engineers, technologists, research students and support staff at NCL for their contributions in "advancement of knowledge and in applying chemical science for good of the people" by way of scientific research and innovations.

A corpus fund made up of contributions from private organizations and individuals interested in NCL's progress and welfare has been created and the earnings from the fund are used to further the objectives of the Foundation. The The NCL RF recognises the contribution of NCL scientists through institution of various awards such as, NCL Foundation Day awards, National Science Day awards and National Technology Day awards to promote excellence in basic science, applied research leading to commercialisation of technology, new initiatives in the R&D support systems, to recognize unusual merit in individuals from the scientific and supporting staff and to promote the safety culture in the laboratory. Besides, it also organises various special lectures in memory/ honour of former NCL Directors.

The NCL Research Foundation has been registered as a public trust and is managed by a Board of Trustees. This Trust has been granted an exemption under the U/S 80G of the Income tax act 1961 to enable it to receive donations.

NCL RF is a unique experiment in public private partnership to encourage all round excellence in all endeavours in the laboratory. It is managed through an independent Board of trustees as a private fund within a public body. It brings to its activities a high level of transparency and accomplishments as well as peer-groups participation in all decision making.

Objectives of the foundation

- To give awards to the teams of NCL scientists, engineers and technologists for scientific innovations or development of commercial technologies of international class. The work must represent a high level of eam effort.
- To give awards, institute fellowships or scholarships, stipends, remuneration and/or other similar payments to NCL scientists and research scholars to facilitate their undertaking a high level of scientific and technological research in the area of interest to NCL.
- To establish and support professions, fellowships, lectureships, scholarships and prizes.
- To award scholarships and fellowships and grants to NCL scientists and research scholars by way of loan and otherwise and on such terms and conditions, as the trustees may think fit for the purpose of undertaking, prosecuting and encouraging research work in Chemistry, Chemical technology, Chemical engineering, Biological sciences And other branches of sciences of interest to NCL.
- To encourage and support participation by NCL scientists and research scholars in the conferences and seminars abroad for activities relating to the research areas of interest to NCL.
- To print, publish and exhibit or subsidies the publication of any pamphlets, or posters relating to the research done by NCL scientists and research scholars.
- To provide for, educate and train NCL staff or other institutes in India or abroad to enable them to manage research and other infrastructural groups effectively.
- To devise incentive schemes, or reward systems for the supporting staff belonging to administration, finance, purchase, marketing and other related sections, so that they can effectively contribute towards the attainment of laboratory's R&D goals.
- To promote, develop and improve scientific exchange of knowledge as well as technical cooperation between research institutions having objects similar to that of the foundation.
- To do all acts, matters and things as are incidental or conducive to the attainment of the above aims and objects or any one or more of them.
- To takeover or amalgamate with other charitable society or trust with similar objects.

Board of trustees

The Board of Trustees consists of members as given below and such other persons as may be appointed from time to time.

- Director, NCL - Ex-officio member & Chairman
- Chairman, Research Council, NCL - Ex-Officio member
- Director, MUDCT - Ex-Officio member
- Two senior most divisional Heads, NCL - Ex-Officio members
- Controller of Administration / AO, NCL - Ex- Officio member.
- Senior Finance & Accounts officer / F&AO, NCL - Ex-Officio member
- One Research Council member
- One representative from industry

The Director, NCL is the Ex-Officio Trustee and the Chairman of the Trust. He/She presides over all meetings of the Trustees. In his/her absence, the person whom the Trustees present at the meeting elect as Chairman of the said meeting by a vote of majority acts as the Chairman of the said meeting.

The Ex-Officio members are the trustees of the Trust by virtue of their post and the person holding the respective post continues as trustee of this Trust till he relinquishes the post or another member is nominated in his place by his organization/ department.

As regards the trustees other than ex-officio members, the tenure does not exceed more than three years. However, the Board of Trustees have the power to extend the tenure of such trustees.

Board of Trustees (2002-2004)

POSITION	PRESENT BOARD	BY VIRTUE OF
Chairman	Dr. S Sivaram	Director, NCL
Member	Prof. M. M. Sharma	Chairman, Research Council
Member	Prof. J. B. Joshi	Director, MUICT
Member	Mrs. S. F. Vakil	Representative of Donor Industry
Member	Mr. Desh Bandhu Gupta	Representative of Donor Industry
Member	Dr. B. D. Kulkarni	Deputy Director, NCL
Secretary	Mr. M. S. Vidyanathan	CoA, NCL
Treasurer	Mr S Chandrahas	SFAO, NCL
Jt. Secretary	Mr. G. Prabhakaran	—

Awards/ Lectures

NCL Research Foundation gives various awards on NCL Foundation Day, National Science Day and National Technology Day, besides organising the special lectures of eminent personalities in honour /memory of former NCL Directors.

NCL foundation day awards

Scientist(s) of the Year Award: This award carries a cash prize of Rs. 20,000/- and a citation to the award winner. The award is peer reviewed by an external committee. The two awards in this category are: "Shirinbai & Maneckji Neterwala Scientist of the Year Award" and "R.A. Mashelkar Scientist of the Year Award".

Technology of the Year Award: This award is funded by ICICI and carries a cash prize of Rs. 30,000/- and a citation. The award is peer reviewed by an external committee.

Highest Industrial Earning Award: This award carries a Trophy and a rotating shield to the winner(s) based on the per capita industrial earning of the division.

New Initiative Taken by the R&D Support System: This award carries a cash prize of Rs. 20,000/- and a Certificate of Merit. The award is given for the group activity and not for individual performances.

Individual Merit Award(s): This award carries a cash prize of Rs. 2500/- each and a Certificate of Merit. There are total six awards - three for scientific staff - and three for technical staff.

Director's Commendation Awards: The Chairman NCL RF recognizes an individual or a group of individuals for their exemplary performance leading to significant accomplishment in any activity of relevance to the laboratory.

National science day awards

Keerti Sangoram Memorial Endowment Award for Best Papers: This award for research students carries a cash of Rs. 2500/- each and a Certificate of Merit for four students in the area of Physical / Material Sciences, Biological Sciences and Chemical Sciences and Engineering Sciences.

Dr. Rajappa award for the best organic chemistry paper: This award for research students carries a cash prize of Rs. 1000/- and a citation.

Best poster awards

National technology day awards

International Patent Award: This award carries a certificate for all the team members for every foreign patent granted.

Lectures

NCL RF organizes several special lectures in memory/ honour of its former Directors All the lectures carry a honorarium of Rs.10,000/- and air travel expenses to the invited speakers. This year NCL RF organised six special lectures.

NCL foundation day awards (2003)

NAME OF AWARD	AWARD	AWARD WINNER(S)	AWARDED FOR
NCL RF Scientist of the Year Award (Sponsored by Maneckji & Shirinbai Neterwala Foundation)	Rs. 20,000/- +Citation	Dr. S. P. Chavan (Organic Chemical Technology Division)	For significant contributions to the synthesis of biologically active compounds and development of novel synthetic methodologies.
NCL RF Scientist of the Year Award (Sponsored by Dr. R.A. Mashelkar Endowment Fund)	Rs. 20,000/- +Citation	Dr. S. Ganapathy (Central NMR Facility)	For significant contributions to the advancement of solid state NMR methods for the study of new materials such as chiral catalysts, polymers and other soft materials.
NCL RF Technology of the Year Award (Sponsored by ICICI Ltd.)	Rs. 30,000/- +Citation	Process for preparation of S(-) amlodipine besylate Dr. R. A. Joshi Dr. (Mrs.) R. R. Joshi (Organic Chemical Technology Division)	For successful development and commercialization of amlodipine process using natural tartaric acid.
Highest Industrial Earning Award	Rotating Shield & Trophy	Polymer Chemistry Division	Highest per capita (net) industrial earning during 2002-03
Award for "New Initiative taken by the R&D Support System"	Rs. 20,000/- each + Certificate of Merit	(Shared Jointly) Project Management Information system (PMIS) Dr. S. Krishnan Mr. G. Prabhakaran Mr. Siddharth Parulikar (Information Division)	For design, development & successful implementation of PMIS, which resulted in project information being made available to the desk top Of scientists.
Award for "New Initiative taken by the R&D Support System"	Rs. 20,000/- each + Certificate of Merit	ncl@home Dr. V. Premnath Mr. K. D. Deshpande Mr. A. D. Kulkarni Mr. Raju Malge Mr. U. V. Dhavale Mr. A. V. Sahasrabudhe	For conceiving, creating and sustaining an institutional portal ncl@home with great imagination and providing a platform for internal communication amongst all the staff of NCL

For enhancing the prestige of NCL through a paper "Ca^{2+} -Keggin colloidal particles as templates for the growth of star-shaped calcite crystal assemblies" which was highlighted in the cover page of **"Langmuir"**	**Director's Commendation Award**	Rs. 5,000/- + Certificate of Commendation	**Dr. Murali Sastry Dr. S. R. Sainkar Mr. D. Rautaray**		
For enhancing the prestige of NCL through a paper "A rational study of crystal engineering of supramolecular assemblies of 1,2,4,5-benzenetetracarboxylic acid" which was highlighted in the cover page of **"Journal of Organic Chemistry"**	**Director's Commendation Award**	Rs. 5,000/- + Certificate of Commendation	**Dr. V. R. Pedireddi Mr. K. K. Arora**		
For exhibiting exemplary presence of mind and timely action, beyond the call of normal duty, during the fire that occurred at NCL in January, 2003	**Director's Commendation Award**	Rs. 1,000/- each + Certificate of Commendation	**Mr. M. S. Vidyanathan Dr. G. S. Grover Mr. S. V. Mohite Dr. M. M. Jana Mr. M. B. Bhavsar Dr. T. P. Mohandas Mr. B. G. Ponkshe Mr. A. V. Mahajan Mr. Jaipal Singh Dr. R. A. Joshi Mr. S. M. Mane Mr.S. P. Burujpatte Mr. V. D. Mindhe**		
For his initiative towards developing conductivity probes and associated signal conditioning unit which has resulted in the development of two professional grade V-probe units for NCL	**Individual Merit Award**	Rs. 5,000/- + Certificate of Merit	**Mr. V. V. Borkar (PSE Group)**		
For his initiative towards follow up with the MSEB to get electricity metering as per power consumption in MERADO & thereby improving the power factor from 0.9 to 0.95. He was ably assisted in this task by Mr. S.M. Mane & Mr. Karanjkar	**Individual Merit Award**	Rs. 5,000/- + Certificate of Merit	**Mr. R. P. Purandare (Engineering Service Unit)**		
For his initiative in planning and execution of activities related to civil and inferior work and thereby completing the renovation of NCL Guest House in a record time. He was ably assisted in this task by Mr. S. M. Mane & Mr. Jaipal Singh	**Individual Merit Award**	Rs. 5,000/- + Certificate of Merit	**Mr. A. V. Mahajan (Engineering Services Unit)**		

NATIONAL SCIENCE DAY AWARDS (2003)

Keerthi Sangoram Memorial Endowment Award for Best Research Fellows

I. Best Papers

Area	Best Research Scholar of the Year-2003	Guide	Award
Physical/Material Sciences (Shared Jointly)	Mr. Joseph Joly V.L.	Dr. P. A. Joy	Rs. 1,250/- + Citation
	Mr. Saikat Mandal	Dr. Murali Sastry	Rs. 1,250/- + Citation
Chemical Sciences	Mr. Anirban Kar	Dr. Narshinha P. Argade	Rs. 2,500/- + Citation
Biological Sciences	Santosh Ramvilas Vyas	Dr. Anil H. Lachke	Rs. 2,500/- + Citation
Engineering Sciences	Mr. Prakash S. Shelokar	Dr. B. D. Kulkarni	Rs. 2,500/- + Citation

II. Dr. Rajappa Prize Award for the Research Students

For the research paper in Organic Chemistry with the highest impact factor	Mr. Nagendra K. Sharma	Dr. K. N. Ganesh	Rs. 1,000/- + Citation

III. Best posters

Biochemical sciences

Biosynthesis of polyhydrosybutyrate and its copolymer by Bacillus Sp., D. Rohini and S.K. Rawal

HIV-1 is a DNA binding transcription factor: role in viral and cellular gene expression, Dineshkumar H. Dandekar

Catalysis

Synthesis of silica functionalised sulphonic acid groups for acid catalyzed reactions, S. Shylesh. Surendran Parambadath, Shrikant S. Bhoware and A.P. Singh

Chemical engineering & process development

Optimization of bilayer polymeric actuator design, S. Radhakrishnan and Swarnendu B. Kar

Small world behaviour of complex reaction networks, Jainy Kuriakose, Anandamohan Ghosh, V. Ravi Kumar and B.D. Kulkarni

Organic chemistry

Towards the design of a perfect catalyst for Pinacol coupling of Ketones, Anamitra Chatterjee

Total synthesis of LG-2/LG-20: A Galactosylmaltotrisaccharides, Mukund K. Gurjar, Bhargava K and C.V. Ramana

Enantioselective total synthesis of (-)-Galantinic acid, Satyendra Kumar Pandey and Pradeep Kumar

Physical & materials chemistry

Electrochemical detection of 14 consecutive Single Electron Charging Steps of 4mm sized Au nanoclusters: Experimental verification of size dependent Kubo Gap, Nirmalya Kumar Chaki, Bhalchandra Kakade, S. Mahima, Jadab Sharma, I.S. Mulla, Renu Pasricha and K. Vijayamohanan

Polymer science

Nitrogen- and Oxygen-containing ansa-Fluorenyl Group IV Metal Complexes: Synthesis and Application as Ethylene Polymerization Catalysts, A. Rajesh, T.P. Mohandas and S. Sivaram

Dateline NCL

The national technology day

(11 May, 2003): NCL celebrated The National Technology Day by organizing Prof. B.D. Tilak memorial lecture. Prof. M.S. Swaminathan, FRS, UNESCO Cousteau Chair in Ecotechnology & Chairman, M.S. Swaminathan Research Foundation, Chennai delivered the Prof. B.D. Tilak memorial lecture on 4th August 2003. In his speech on "Science and Sustained Agriculture Progress" Prof. Swaminathan urged to foster an ever-green revolution based on principles of ecology, gender and social equity, economics, employment generation, and energy conservation.

Prof. K. Venkataraman memorial lecture

(19 August, 2003): Prof. Goverdhan Mehta, Director, Indian Institute of Science, Bangalore delivered the second Prof. K. Venkataraman Memorial Lecture on "Design of new molecular objects: art & logic in organic synthesis".

Hindi week

(8-15 September, 2003): NCL observed "Hindi week" by organising various competitions for staff members, to promote the use of Hindi in their day-to-day work, were organized during the week. *"NCL Alok"*, a Hindi Annual Bulletin was also released.

CSIR foundation day

(27 September, 2003): Prof. S.K. Joshi, former Director General, CSIR delivered CSIR Foundation Day lecture on "CSIR: 60 Years Behind and 60 Years Ahead". Looking at the past of CSIR, Prof. Joshi said these sixty years had been very eventful and turbulent for CSIR. Prof Joshi also elaborated on his perspectives of CSIR for the next 15 years.

Prof. J.W. McBain memorial lecture

(7 October, 2003): Prof. Ajay Sood, Department of Physics, Indian Institute of Science, Bangalore delivered the third Prof JW McBain memorial lecture on "Carbon Nanotubes: Paradigm for New Science and Technology".

Vigilance week

3-8 October, 2003): NCL observed vigilance week to create awareness among the staff members. The events like essay writing and debate contest on "Advantages of transparency in official dealings" and "Whether anti-corruption measures adopted by Government machinery are adequate to deal with unethical activities by anti-social elements", respectively, were organized to make members of the staff aware about the rules and regulations which required attention as also the transparency in day-to-day work. The programmes were well attended. Shri V.M. Bhandari, Supdt. Engineer, Vigilance & Quality Control, PWD Office addressed the staff members. The talk was informative and well appreciated.

Nobel evening 2003

(16 October, 2003): CRSI (Pune Chapter) organized a Nobel Evening 2003 at NCL. Presentations were given by NCL scientists on the Nobel Prizes winning work in Chemistry, Physics and Physiology & Medicine.

CPYLS

(13-14 November, 2003): NCL being a coordinating laboratory to implement CSIR Programme on CPYLS in Maharashtra organised a two-day a counseling session and lectures. About 100 meritorious students accompanied with their teachers and parents participated in the programme. Besides, about 300 invited students of class XI and XII from local schools also attended the inaugural session of the function. Prof. Arvind Gupta from Inter-University Centre for Astronomy and Astrophysics (IUCAA), *Muktangan* Science Centre, Pune delivered a keynote address on "fun of science". Ms. Gayatri Natu and, Mr. Niraj Deosthali, who are pursuing their career in natural science at IIT Kanpur and Ruparel College, Mumbai, respectively, and were participants of CPYLS counseling programme at NCL held in 2000, were conferred under-graduation level CSIR Student Associateship.

INSA AGM

(27-28 December, 2003): NCL organized 69th Anniversary General Meeting of Indian National Science Academy (INSA). Dr R.A. Mashelkar, Director General, CSIR launched e-Journal portal of the INSA.

NCL foundation day

(3 January, 2004): Professor Madhav Gadgil, Centre for Ecological Sciences, Indian Institute of Science, Bangalore delivered the NCL foundation day lecture on "Engaging people in conserving nature". NCL celebrated its fifty-fourth foundation day on 3rd January, 2004. Several NCL Research Foundation awards including scientist of the year award, technology of the year award, highest industrial earning award and individual merit award were given away by Prof. Gadgil.

Invited lecturer

(27 January, 2004): Prof. Philip Cohen, FRS, FRSE, Director of Medical Research Council Protein Phosphorylation Unit, Director of the Wellcome Trust Biocentre and Director of Research at School of Life Sciences, University of Dundee, Scotland (UK) delivered a talk on "Kinase inhibitors: Drugs for 21st Century".

Dr. L.K. Doraiswamy lecture

(17 February 2004): Professor Frederick J. Krambeck, Johns Hopkins University, Whiting School of Engineering, USA delivered Dr. L.K. Doraiswamy Lecture in Chemical Engineering on "Glycosylation Reaction Kinetics".

National science day

(27-28 February, 2004): The student community of NCL organised a two-day programme to celebrate the National Science Day. The programme included poster presentations by Research Students, Presentations by CSIR Young Scientist awardees, Keerti Sangoram Awardees in Chemical Sciences, engineering sciences, physical & Material Science and Biological Sciences, and by Dr. Rajappa awardee for Research Paper in Organic Chemistry. About 150 posters were displayed by the research students covering the chemistry, and allied sciences. Prof. Ashoke Sen, FRS, Harish Chandra Research Institute, Allahabad delivered a Science Day Lecture on "Search for a Unified Theory".

National safety day

(10 March, 2004): Various programmes like fire-fighting demonstration, presentation of safety plan for 2004-05 by Chairman, Safety Committee, film-show on Chemical & Fire Safety were organised. A special talk by Dr. T. Rajgopal, Corporate Medical Advisor, Hindustan Lever Limited, Mumbai on "Occupational Health, Safety & Environment Management in a chemical laboratory" was also organised. Safety conveners of various Divisions presented their divisional safety reports.

Dow endowment lecture in honour of Dr Paul Ratnasamy

(11 March 2004): Prof Wolfgang F. Holderich, Director, Chemical Technology and Heterogeneous Catalysis, University of Technology, RWTH Aachen, Germany delivered the first Dow Endowment lecture in honour of Dr Paul Ratnasamy, former Director of NCL. Prof. Holderich spoke on "New Heterogeneously Catalyzed Processes for Environmentally Benign and Sustainable Chemical Production".

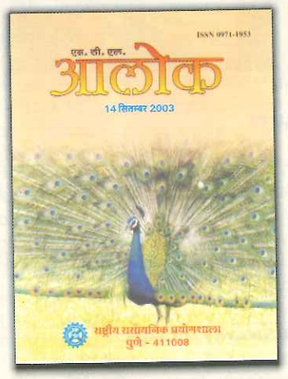
राजभाषा का कार्यान्वयन

राष्ट्रीय रासायनिक प्रयोगशाला में रसायन विज्ञान एवं रासायनिक अभियांत्रिकी के क्षेत्र में अन्तर्राष्ट्रीय स्तर के शोधकार्य किए जाते हैं । इस प्रयोगशाला में दैनिक कामकाज में राजभाषा के प्रयोग को भी बढ़ावा दिया जाता है । चूँकि यह एक अनुसंधान प्रयोगशाला है, अत: यहाँ 75 प्रतिशत कार्य वैज्ञानिक एवं तकनीकी स्वरूप का एवं शेष 25 प्रतिशत कार्य प्रशासनिक स्वरूप का होता है । प्रशासनिक स्वरूप के कार्य का अधिकांश भाग हिन्दी में संपादित किया जाता है । राजभाषा अधिनियम की धारा 3 (3) के अन्तर्गत जारी होने वाले सभी दस्तावेज अनिवार्य रूप से हिन्दी तथा अँग्रेजी दोनों में साथ साथ जारी किए जाते हैं । हिन्दी में प्राप्त पत्रों के उत्तर हिन्दी में ही दिए जाते हैं । राजभाषा कार्यान्वयन समिति की बैठकें प्रत्येक तिमाही में नियमित रूप से होती हैं, जिनमें हिन्दी के प्रगामी प्रयोग की समीक्षा की जाती है । सभी रबड़ की मोहरें, पत्र-शीर्ष, फॉर्म तथा मानक मसौदे द्विभाषी बना लिए गए हैं । सभी साइनबोर्ड द्विभाषी बने हुए हैं । प्रयोगशाला के मुख्य कम्प्यूटर सर्वर में द्विभाषी सॉफ्टवेयर ''लीप ऑफिस-नेटवर्क वर्ज़न'' स्थापित करके कम्प्यूटरों को द्विभाषी बना दिया गया है । निदेशक महोदय का स्टाफ को सम्बोधित पत्र प्रत्येक तिमाही में अँग्रेजी के साथ-साथ हिन्दी तथा मराठी में भी जारी किया जाता है।

प्रयोगशाला में टिप्पण एवं आलेखन सम्बन्धी प्रोत्साहन योजना लागू है । प्रयोगशाला के रोकड़ अनुभाग तथा अल्पाहारगृह के कार्यालय में समस्त कार्य हिन्दी में ही किया जाता है । **क** तथा **ख** क्षेत्रों को जाने वाले अधिकांश पत्रों के लिफाफों पर पते हिन्दी में ही लिखे जाते हैं । हिन्दी का कार्यसाधक ज्ञान रखने वाले कर्मचारियों के लिए नियमानुसार हिन्दी कार्यशालाओं का आयोजन किया जाता है । **एनसीएल आलोक** नामक वार्षिक हिन्दी गृहपत्रिका का प्रकाशन नियमित रूप से किया जाता है । भारत सरकार के जैवप्रौद्योगिकी विभाग के सौजन्य से प्रयोगशाला ने हिन्दी में **वसुन्धरा का हरित परिधान** नामक एक वृत्त चित्र (डॉक्युमेंटरी फिल्म) का भी निर्माण किया है ।

प्रयोगशाला में प्रतिवर्ष हिन्दी दिवस/हिन्दी सप्ताह मनाया जाता है । इस उपलक्ष्य में विभिन्न प्रतियोगिताओं एवं सांस्कृतिक कार्यक्रमों का आयोजन किया जाता है । इसके अलावा सी.एस.आई.आर. मुख्यालय की मौलिक (विज्ञान) पुस्तक लेखन योजना, वैज्ञानिक कार्यों में हिन्दी पुरस्कार योजना तथा विज्ञान चिन्तन लेखमाला आदि योजनाओं में प्रयोगशाला के वैज्ञानिक एवं कर्मचारी भाग लेते हैं । इन योजनाओं में वैज्ञानिकों एवं कर्मचारियों को पुरस्कार भी प्राप्त हुए हैं । प्रयोगशाला के लगभग 90 प्रतिशत कर्मचारियों को हिन्दी का प्रशिक्षण दिया जा चुका है । शेष कर्मचारियों को भी प्रशिक्षित करने की प्रक्रिया जारी है । चूँकि प्रयोगशाला के 80 प्रतिशत कर्मचारियों को हिन्दी का कार्यसाधक ज्ञान प्राप्त है, अत: इसे राजभाषा नियम, 1976 के नियम 10 (4) के अधीन राजपत्र में अधिसूचित किया जा चुका है ।

प्रयोगशाला वैज्ञानिक अनुसंधान के क्षेत्र में राजभाषा के प्रगामी प्रयोग की दिशा में भी सजग है । यहाँ के वैज्ञानिक देश के विभिन्न संस्थानों में राजभाषा के माध्यम से आयोजित होने वाले राष्ट्रीय विज्ञान सम्मेलनों/संगोष्ठियों में भाग लेकर हिन्दी में अपना शोधपत्र प्रस्तुत करते हैं । प्रशोगशाला में भी राजभाषा के प्रयोग को बढ़ावा देने के लिए समय-समय पर हिन्दी माध्यम से विज्ञान संगोष्ठियों एवं कार्यशालाओं का आयोजन किया जाता है ।



प्रयोगशाला में हिन्दी सप्ताह समारोह का आयोजन

राष्ट्रीय रासायनिक प्रयोगशाला, पुणे में दि. 8-15 सितम्बर, 2003 तक **हिन्दी सप्ताह समारोह** का आयोजन किया गया । इस उपलक्ष्य में प्रयोगशाला के स्टाफ हेतु विभिन्न प्रतियोगिताओं का आयोजन किया गया । समारोह के पहले दिन अर्थात 8.9.2003 को हिन्दी नोटिंग एवं ड्राफ्टिंग प्रतियोगिता का आयोजन किया गया । इसमें लगभग 15 कर्मचारियों ने भाग लिया । दिनांक 9.9.2003 को हिन्दी वाद-विवाद प्रतियोगिता आयोजित की गई । इस प्रतियोगिता में स्टाफ के 12 सदस्यों ने भाग लिया । तत्पश्चात दिनांक 10.9.2003 को हिन्दी निबन्ध तथा 11.9.2003 को हिन्दी श्रुतलेखन प्रतियोगिताओं का आयोजन किया गया । इन प्रतियोगिताओं में कुल 50 कर्मचारियों ने भाग लिया । हिन्दी दिवस के उपलक्ष्य में दि. 12 सितम्बर, 2003 को प्रयोगशाला की वार्षिक राजभाषा पत्रिका, **एन.सी.एल. आलोक** का लोकार्पण किया गया । इस अवसर पर राष्ट्रीय रक्षा अकादमी, पुणे के कुल सचिव एवं हिन्दी विभाग अध्यक्ष, डॉ. मदन मोहन मिश्र मुख्य अतिथि के रूप में उपस्थित थे । उन्होने अपने सम्बोधन में राजभाषा के महत्व पर बल देते हुए कर्मचारियों का आवाहन किया कि वे अपने सरकारी कामकाज में अधिकाधिक हिन्दी का प्रयोग करके राष्ट्र के निर्माण में अपना सहयोग दें । इस समारोह की अध्यक्षता प्रयोगशाला के निदेशक, डॉ. एस. शिवराम ने की ।

दिनांक 15.9.2003 को अपराह्न 4.00 बजे **हिन्दी सप्ताह समापन समारोह** का आयोजन किया गया । समारोह का प्रारंभ सरस्वती वन्दना से हुआ । इस अवसर पर पुणे नगर राजभाषा कार्यान्वयन समिति के अध्यक्ष तथा आयकर अपीलीय अधिकरण, पुणे के न्यायिक सदस्य, श्री यू. बी. एस. बेदी मुख्य अतिथि तथा डॉ. अरुण पुजारी, हिन्दी विभाग अध्यक्ष, फर्ग्युसन कॉलेज, पुणे विशिष्ट अतिथि के रूप में उपस्थित थे । अपने सम्बोधन में श्री बेदी ने इस बात पर दु:ख व्यक्त किया कि आज सरकारी दफ्तरों में राजभाषा में काम नहीं हो रहा है । उन्होंने कर्मचारियों से अनुरोध किया कि वे इस पर गंभीरता से ध्यान दें और भारतीय भाषाओं के विकास को प्राथमिकता देते हुए हिन्दी दिवस को सार्थक बनाएँ । डॉ. पुजारी ने समारोह में उपस्थित कर्मचारियों को सम्बोधित करते हुए कहा कि आज चीन, जापान, फ्राँस और जर्मनी आदि विकसित देशों में वहाँ की राष्ट्रभाषा में ही कामकाज होता है । इन देशों ने अपनी भाषा को ही अपनाते हुए अपना विकास किया है । अत: हमें भी अपनी राष्ट्रभाषा को अपनाकर अपनी अलग राष्ट्रीय पहचान बनानी होगी । उन्होंने सरकारी कामकाज एवं दैनंदिन जीवन में हिन्दी के महत्व को रेखांकित किया ।

इस अवसर पर प्रयोगशाला के उप निदेशक, डॉ. आर. वी. चौधरी अध्यक्ष के रूप में उपस्थित थे । इस समारोह में हिन्दी सप्ताह के उपलक्ष्य में आयोजित हिन्दी प्रतियोगिताओं के विजेताओं को मुख्य अतिथि ने पुरस्कार प्रदान किए । प्रयोगशाला के प्रशासन नियंत्रक, श्री एम. एस. वैद्यनाथन ने धन्यवाद ज्ञापित किया । इसके पूर्व प्रयोगशाला के वरिष्ठ हिन्दी अधिकारी, डॉ. रमाशंकर व्यास ने सभी का स्वागत करते हुए समारोह के महत्व पर प्रकाश डाला । समारोह का संचालन हिन्दी अधिकारी, श्री उमेश गुप्ता ने किया ।

Committees

Scientists, in addition to their research and development functions, also give their valuable time for effectivly managing various activities in the laboratory. The committees are charged with the responsibility of effective utilisation and management of available resources and to ensure wider participation of scientists and staff in decision making in the laboratory.

Statutory committees

Committee	Chairperson
Building and construction committee	Dr. P.V. Rao
Canteen affairs committee	Dr. C.R. Rajan
Colony affairs committee	Dr. M.K. Gurjar
Compassionate appointment committee	Dr. B.D. Kulkarni
Confirmation and probation committee	Dr. R.V. Chaudhari
Grievance committee	Dr. K.N. Ganesh
Information and library committee	Dr. M.G. Kulkarni
ISTAG committee	Dr. R.V. Chaudhari
Medical services committee	Dr. (Mrs) Vidya Gupta
Normalisation committee for APAR grading for technical officers in group iii)	Dr. B.D. Kulkarni
Official language implementation committee	Dr. S. Sivaram
Patents committee	Dr. R.V. Chaudhari
Staff quarter allotment committee	Dr. B.D. Kulkarni
Standing committee for recommending distribution of income from intellectual property, fee for contract R&D and S&T	Dr. B.D. Kulkarni
Standing committee on laboratory safety	Dr. S. Sivaram
Standing disposal committee	Dr. R.V. Chaudhari
Standing purchase committee - I	CoA
Standing purchase committee - II and sub-committees of standing purchase committee	Dr. Ganesh Pandey/ Dr. D.V. Gokhale
Write-off committee	Dr. R.A. Joshi

Institutional/ ad-hoc committees

Committee	Chairperson
Advisory committee for center for materials characterisation	Dr. R.V. Chaudhari
Committee to advise the director on the aspects relating to upkeep, maintenance and upgradation of NCL guest house	Dr. S Devotta
Committee to examine comprehensively the future communications and conferencing needs of NCL	Ms. Neelima Iyer
Committee to examine holistically the current and future needs of NCL's information technology resources	Dr. V. Premnath
Committee to prioritise major equipment purchase from CSIR/ laboratory reserve funds	Dr. K.N. Ganesh
Coordinating committee for central NMR facility	Dr. K.N. Ganesh
Human resource development and management committee	Dr. S. Sivaram
Monitoring committee on stores management	Dr. M.G. Kulkarni
Student affairs committee	Dr. K.N. Ganesh

Research council

up to 31st December, 2003

Chairman
Prof. M.M. Sharma,
Kothari Research Professor,
Former Director, UDCT,
Mumbai 400 071.

Members

Dr. Joseph Thomas,
Director,
SPIC Science Foundation,
Chennai 600 032.

Prof. B. Viswanathan,
Department of Chemistry,
Indian Institute of Technology,
Chennai 600 036.

Dr. Biman Bagchi,
Solid State & Structural
Chemistry Unit,
Indian Institute of Science,
Bangalore 560 012.

Dr. Animesh Chakravorty,
INSA Research Professor,
Department of Inorganic
Chemistry,
Indian Associate for
Cultivation of Science,
Kolkatta 700 032.

Dr. M. Ganapathi,
Incharge Atomic Plant,
Reliance Petroleum Ltd.,
Jamnagar 361140.

Mr. C.N. Trivedi,
Executive Director,
Gas Authority of
India Limited,
New Delhi 110 016.

President,
Indian Chemical
Manufacturers Association,
Mumbai.

Director,
Central Salt & Marine
Chemicals Research Institute,
Bhavnagar 364 002.

Dr. S. Sivaram,
Director,
NCL

DG's Nominee
Director,
Centre for Biochemical
Technology,
Delhi 110 007.

Member Secretary
Dr. K.N. Ganesh,
Head,
Organic Chemistry (Synthesis) Division,
NCL

(1.1.2004 to 31.12.2006)

Chairman
Prof. M.M. Sharma
2/3, Jaswant Baug, Behind Akbarallys,
VN Purav Marg, Chembur, Mumbai 400071.

Members

Prof. S. Chandrasekaran
Department of Organic Chemistry,
Indian Institute of Science,
Bangalore 560 012.

Prof. Ajay Kumar Sood
Chairman,
Department of Physics,
Indian Institute of Science,
Bangalore 560 012.

Prof. M.S. Ananth,
Director,
Indian Institute of Technology,
Chennai 600 036.

Dr. K.V.S. Rao
Head, Immunology Group,
International Centre for Genetic
Engg. & Biotechnology,
ICGEB Campus, Aruna Asaf Ali Marg,
New Delhi 110 067.

Shri Sujit Banerjee,
Senior Vice President, (Polymer)
Planning Research and Business
Development, RIL, Reliance Centre,
19, Walchand Hirachand Marg,
Ballard Estate, Mumbai 400 038.

Dr. J.M. Khanna,
Executive Director and President,
Jubilant Organo Systems Ltd.,
1-A, Sector 16-A, Institutional Area,
Noida 201 301.

Dr. G.N. Qazi,
Director,
Regional Research Laboratory,
Canal Road, Jammu 181 001

Dr. S. Sivaram,
Director,
NCL

DG's Nominee
Dr. J.S. Yadav,
Director, Indian Institute of Chemical
Technology, Uppal Road,
Hyderabad 500 007.

Permanent Invitee, President of ICMA
Mr. Deepak Mehta,
Managing Director,
Deepak Nitrite,
National Games Road,
Shastri Nagar, Yerawada, Pune

Permanent Invitee, CSIR
Dr. O. P. Agarwal
Head, R&D Planning Division,
CSIR, Anusandhan Bhawan,
2, Rafi Marg, New Delhi 110 001.

Member Secretary
Dr. G.S. Grover,
Head, Research Planning & Audit Unit,
NCL

Management council

MANAGEMENT COUNCIL
[1.7.2001 TO 30.6.2003]

Chairman:
Dr. S. Sivaram,
Director, NCL

Member-Secretary:
Mr. M.S. Vidyanathan,
Controller of
Administration, NCL

Members

Dr. B.D. Kulkarni,
Deputy Director, NCL

Dr. S. Devotta,
Scientist, NCL

Dr. R.R. Hirwani,
Head, RPBD, NCL

Dr. (Mrs.) Mala Rao,
Scientist, NCL

Dr. Murli Sastry,
Scientist, NCL

Dr. A.A. Kelkar,
Scientist, NCL

Mr. R.P. Purandare,
Technical Officer 'B', NCL

Mr. S. Chandrahas,
Senior F & A O, NCL

MANAGEMENT COUNCIL
[1.7.2003 to 30.6.2005]

Chairman:
Dr. S. Sivaram, Director,
NCL

Member-Secretary:
Mr. M.S. Vidyanathan,
Controller of
Administration, NCL

Members

Dr. B.D. Kulkarni,
Deputy Director, NCL

Dr. R.V. Chaudhari,
Scientist, NCL

Dr. (Mrs.) V.V. Deshpande,
Scientist, NCL

Dr. V.V. Ranade,
Scientist, NCL

Dr. K. Vijaymohanan,
Scientist, NCL

Mr. G. Prabhakaran,
Scientist, NCL

Mr. D.B. Pradhan,
Technical Officer, NCL

Mr. S. Chandrahas,
Senior F&AO, NCL

National Chemical Laboratory

V. Ranade bags SS Bhatnagar Prize in Engineering Sciences for the yea

ABOUT NCL
RESEARCH GROUPS
RESOURCE CENTERS
FACILITIES
ACHIEVEMENTS

Your Partner from

NCL, India is a research, development and consulting organisation with a focus on chemistry and chemical engineering. It has a successful record of research partnership with industry.

R&D Feature

Cholesterol removal

more >>

- Tenders
- Licensing & Services
- NCIM
- Job Vacancies

Reports & Press Releases

- Celebration of CSIR Foundation Day at NCL
- Hydrogen based fuel cell

more >>

NCL in News

- NCL walks wild side to catalogue Indian animals (Times of India, 28 October, 2004)
- Database: Beyond the Jungle Book (Science, 22 October 2004)

more >>

Major Events

- Annual general meeting of Materials Research Society of India
- A one-day Symposium on Complex Fluids

more >>

National Chemical Laboratory (NCL)
Dr. Homi Bhabha Road, Pune - 411008,India
EPABX:+91(0)20-25893300;**Fax:**+91(0)20-25893619
Email:pki@ems.ncl.res.in; **Gram:** CHEMISTRY, PUNE

Last Updated Date : 01-Nov-2004

राष्ट्रीय रासायनिक प्रयोगशाला
डॉ. होमि भाभा मार्ग, पुणे - 411 008 . भारत

NATIONAL CHEMICAL LABORATORY
(Council of Science & Industrial Research)
Dr. Homi Bhabha Road, Pune - 411 008. India
Tel. : +91-20-2589 3300 / 3400
URL : www.ncl-india.org