A Ph.D. Thesis on

SIMULATION AND OPTIMIZATION OF CHEMICAL PROCESS PLANTS

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BY

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September 2014

CERTIFICATE

This is to certify that, the work incorporated in the thesis entitled "**SIMULATION AND OPTIMIZATION OF CHEMICAL PROCESS PLANTS**", submitted by Mr. Ratnadip R Joshi, for the Degree of Doctor of Philosophy in Chemical Engineering at University of Pune, was carried out by him under the supervision of Dr. B D Kulkarni, Distinguished Scientist-CSIR; at Chemical Engineering and Process Development Division, CSIR-National Chemical Laboratory, Pune – 411 008, India.

September 05, 2014

Director,
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September 05, 2014

Dr. B. D. Kulkarni
Research Guide

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LIST OF ABBREVIATIONS and SYMBOLS USED

A	Cross-sectional area of the fluidized bed, $A = (1/4)*\pi*D^2$ m^2
A, B, C	Heat capacity coefficients
A_1, A_2, A_3	Frequency factors for Arrhenius equations
APM	Administered Price Mechanism
ASU	Air separation unit
C_{pg}	Specific heat of gas, J/(kg K)
CAGR	Compound annual growth rate
CC	Combined cycles
CCP	Combined Cycle Plant
CFC	Chloro fluro carbons
D	Diffusion coefficient of gas in emulsion, m^2 /s
D	Nominal diameter of screw in meter
Dt	Bed diameter, m
dB	Mean equivalent bubble diameter, m
d_{BO}	Initial bubble diameter at the surface of the perforated plate, m
d_{BM}	Bubble diameter if there were a single train of bubbles rising along the centre line of the bed, m
Dp	Mean diameter of the particles, m
E_1, E_2, E_3	Activation energies for reactions
E_s	Specific energy, kcal/kg
FCR	Fuel Consumption Rate, kg/hr
FSNL	Full Speed No Load
F-T	Fischer-Tropsch synthesis
g	Acceleration of gravity, m/s^2
ΔG_f	Gibbs free energy of formation

GAIL	Gas Authority of India Limited
GDP	Gross Domestic Product
GRG	Generalized reduced gradient
GT	Gas turbine
GTG	Gas turbine generator
H	Bed height, m
ΔH_f	Standard enthalpy of formation
H_{bc}	Heat transfer coefficient bubble-cloud per unit bubble volume, J/(msK)
H_{mf}	Minimum fluidization height
H_{be}	Heat transfer coefficient bubble-emulsion per unit bubble volume, J/(msK)
H_{ce}	Heat transfer coefficient cloud-emulsion per unit bubble volume, J/(msK)
HC	Hydrocarbon
H.P. Factor	Horsepower Factor
HRSG	Heat Recovery Steam Generator
HTRI	Heat Transfer Research Incorporation®
H_{Vf}	Heating Value of fuel, Kcal/kg
IEA	International Energy Agency
IGCC	Integrated gasification combined cycles
K_i	Rate constants for reaction i
K_{bc}	Mass transfer coefficient bubble-cloud per unit bubble volume, l/s
K_{be}	Mass transfer coefficient bubble-emulsion per unit bubble volume, l/s
K_{ce}	Mass transfer coefficient cloud-emulsion per unit bubble volume, l/s
K_g	Heat conductivity of gas J/(m s K)
K_p	Temperature-dependent equilibrium constant for the CO shift

	reaction
L	length L of the screw conveyor
I_m	Mass flow rate in t/hr
λ	Progress resistance coefficient
LHV	Lower heating value
LNG	Liquefied natural gas
NTPC	National Thermal Power Corporation Limited
LP	Linear programming
M_f	Mass of Fuel, kg
MILP	Mixed integer linear programming
MMBTU	million BTU
MNRE	Ministry of New and Renewable Energy, Government of India
Mtoe	Million Tonnes of Oil Equivalent
NELP	New Exploration Licensing Policy
NGCC	Natural Gas Combined Cycle
NLP	Nonlinear programming
NSM	Jawaharlal Nehru National Solar Mission
NSSO	National Sample Survey Office
OECD	Organization for Economic Cooperation and Development countries
ONGC	Oil and Natural Gas Corporation
p	Partial pressure
PFD	Process Flow Diagram
PRV/PCV	Pressure Regulating /Control Valve
P_H	Power necessary for the progress of the material
P_N	Driving power of the screw conveyor at no load
Q	Volumetric flow rate, m^3/hr

Q_n	Energy needed, kcal/hr
R_f	Forward reaction rate
R_r	Backward reaction rate
RPM	Revolution per minute
RIL	Reliance Industries Limited
SA	Stoichiometric air of fuel
SEBs	State Electricity Boards
SGR	Specific Gasification Rate of Biomass
SLP	*Successive linear programming*
ST	Steam turbine
SQP	*Successive quadratic programming*
Syngas	Synthesis gas
T	Gasifying time, hr
TPES	Total Primary Energy Supply
U_b	Absolute velocity of the bubble phase gas, m/s
U_{br}	Velocity of rise of a single bubble, m/s
U_{mf}	Minimum fluidization velocity, m/s
U_o	Inlet gas velocity, m/s
U_e	Velocity of emulsion gas, m/s
UMPP	Ultra Mega Power Plants
v	Volume fraction
V_S	Superficial gas Velocity, m/s
VB	Visual Basic
Z*	Bubble position (height) in the bed, m
δ*	Fraction of bubble phase volume in fluidized bed
ε	Voidage of the emulsion phase
ε_{mf}	Value of *E* at minimum fluidizing conditions

ξ_g	Gasifier efficiency, %
φ	Sphericity
ρ	Fuel density, kg/m^3
ρ_a	Air density, 1.25 kg/m^3
ρ_f	Air density to the temperature and pressure operation conditions of the gasifier
ρ_p	Particle density in $kg.m^{-3}$
μ	Air viscosity to the temperature and pressure operation conditions of the gasifier

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DECLARATION

I, Mr. Ratnadip R Joshi, hereby declare that this thesis entitled “Simulation and Optimization of Chemical Process Plants” submitted by me for the Degree of Doctor of Philosophy in Chemical Engineering under Faculty of Engineering at University of Pune is the record of bonafide work carried out by me at Chemical Engineering and Process Development Division of CSIR-National Chemical Laboratory, Pune, India, under the guidance of Dr. B. D. Kulkarni. The thesis has not formed the basis for the award of any Degree, Diploma, Associate ship, Fellowship, Titles in this or any other University or other institutions of higher education. I further declare that the material obtained from other sources have been duly acknowledged in the thesis.

Ratnadip R Joshi

SIMULATION AND OPTIMIZATION OF CHEMICAL PROCESS PLANTS

Abstract

According to the current trends and predictions till the year 2035, the world energy consumption will increase at a rate of 1.4 % per year. The global recession that started in the year 2008 had a significant impact on the GDP and energy consumption throughout the world. During this, growth in global energy consumption slowed to 1.2 % in 2008 and declined by around 2.2% in 2009. The trend continued till mid 2013. Although, some improvements are seen in the first two quarters of 2014, i.e. till June 2014. Historically, the Organization for Economic Co-operation and Development (OECD) member countries have accounted for the largest share of current world energy consumption. This trend reversed 2007 and the energy use among non-OECD nations exceeded that among OECD nations. The discrepancy between OECD and non-OECD energy use will grow in future due to the more rapid growth in energy demand expected for the emerging non-OECD economies. Strong dependency on crude oil, natural gas and the associated price and supply chain risk emerges the need for efficient utilization of existing non-renewable energy sources (*e.g.*, coal, natural gas, nuclear power, etc.). The emission of different pollutants, especially green house gases, may urge the environmental regulations to be a strong driver for new developments This is a challenge for decision makers that regulate the energy policies of states and regions, in particular. In this context, coal and biomass have to be considered as energy source for power generation because of availability and relatively wide geographic distribution.

The chemical industry has undergone significant changes during the past 25 years due to the increased cost of energy, increasingly stringent environmental regulations, and global competition in product pricing and quality. One of the most important engineering tools for addressing these issues is modeling, simulation and optimization. Modifications in plant design

and operating procedures have been implemented to reduce costs and meet constraints, with an emphasis on improving efficiency and increasing profitability. Optimal operating conditions can be implemented via increased automation at the process, plant, and company levels. As the power of computers has increased, the size and complexity of problems that can be solved by optimization techniques have correspondingly expanded.

The present study also works on the theme of Simulation and Optimization of Chemical Process Plants with specific focus on energy sector. The need of power and energy security of world as well as that of India is elaborated in chapter 1. Enhanced modeling and optimization for a natural gas based power plant for capacity enhancement was the principle study driving force. A simulation and optimization study was successfully carried out on this power plant. This 93 MW power producing plant was optimized to produce 131 MW power without drastic changes into the plant, which were heavily capital intensive. The detailed methodology implemented is explained in chapter 2. This success triggered to think on enhancement of existing fluidized bed coal gasifiers to optimize their efficiency. The design, modeling, simulation and optimization of the fluidized bed gasifier are detailed in chapter 3. As inefficiencies in gasifiers were observed and the residence time shortcomings were noted, an innovative design of horizontal feeder gasifier is presented in chapter 4. The novelty of the work is illustrated with design and optimization of a horizontal feeder gasifier. Considering the acute shortage of petroleum feedstock, in general, and good quality of fuel, in particular, chapter 5 provides solution on difficulties faced by present energy industry sector by providing simulations for combined feed power plants. As combined cycle power plants in the form of IGCC are being implemented in practice very recently, combined feed is a new form and remedy suggested to the world energy sector through the present study by the present authors. Now, with all the enhancements and optimization in coal, natural gas and combined feed gasifiers along with innovative horizontal feeder gasifier suggested, a newer development for usage of biomass in power plant is studied through chapter 6. Applying modeling, simulation and optimization tools to large scale biomass based power plants is not reported yet in the scientific community and hence we claim the novelty of the work for the present study.

In all, every chapter introduces a new concept for overcoming real industry difficulties, converts them into opportunities, and suggests innovative and practically implementable solutions on such opportunities.

The objectives and outcomes of each chapter are briefly discussed below.

Chapter 1 provides a brief introduction about design, modeling, simulation and optimization tool Aspen HYSYS® from AspenTech, Inc. This is the largest applied simulation tool in the world and many revamping and optimization scenarios are built by extensive use of this simulator. Chapter 1 also provides information on availability and need of energy security as the applied topic of the present study. The collective information emphasizes the immediate need and attention of researchers to provide efficiency enhancement techniques to the world along with newer energy resources and technology as a long term goal. The present researchers have chosen this as the opportunity to work in the energy sector and apply the modern tools for the benefit of masses.

An optimization scheme is presented in chapter 2 for the power plant through process simulation and sensitivity analysis of the key operating parameters. Then, a heat integration scheme is presented for different sections of the process. The newly installed fuel gas system has the capacity to deliver 55360 Nm^3/hr of fuel gas flow. The design capacities of various units of fuel gas system are however limited to 47400 Nm^3/hr. Full utilization and maximum power generation will require drastic design changes. Presently the fuel supply is constrained to a limit of 35630 Nm^3/hr due to limited availability of feed stock raw material. All calculations are therefore carried out for this limiting case. Fuel supply modifications such as by passing the heater skid saves energy on heating the gas to the tune of 900 kWh electric power. Maximum possible power generation in four GTGs is approximately 131 MW. The existing power plant could produce only 93 MW with 31 MW each for three GTGs, having 100 MW as rated design capacity.

This basic study in chapter 3 investigates bed fluidization and particle decomposition for fluidized materials. Effects of particle density and diameter on the minimum fluidization velocity were investigated; a method was developed to predict hydrodynamic response of binary beds from the response of each particle type and mass. This report contains calculations and results of minimum fluidization velocity, fluidization velocity (Uf), cross sectional area, volumetric flowrates, minimum fluidization height, TDH, total height of the column along with bubble dynamics.

Innovative design of horizontal feeder gasifier is presented in chapter 4. Other study components of present report provides real plant data optimization techniques where as this chapter suggests a complete new approach for gasifier design. Horizontal feeder gasifier is used to reduce the limitations of direct feed injection mechanism. Horizontal feeder gasifier increases the retention time which will help to increase the reaction efficiency. Introduction of horizontal feeder before the gasifier cleans the feedstock by ash removal and waste particle removal. Preheating of the coal helps in attaining the equilibrium state of reaction in the gasifier reducing chances of non ideality. A process optimization method has been developed and applied to study the coal gasification for the production of synthesis gas. The boundary definition and the identification of main units are basic steps for the process analysis. Thermodynamic databases, parametric models and steady state simulation are fundamental tools, which are appropriately combined to gain the specific advantages**.**

Chapter 5 is another innovative approach to resolve the scarcity of one type of fuel and reduce dependency of power plants on specific fuels. This has been a reason that many power stations are not producing to their capacity as fuel like coal of good quality is not available as of requirement. As with any fuel like natural gas or naphtha, over dependency because of the energy that it is able to provide by virtue of its calorific value, is inevitable. As a result, depletion of a particular fuel becomes a consequence. Therefore, steps are taken these days to check for the viability of other fuels that may/can be used in combination with one another in order to overcome this limitation. The purpose of this study is meant to serve moves beyond the idea expressed above. In this sense, we have focused on power generation from an IGCC plant by allowing the syngas that comes out of the gasifier to blend itself in the following configurations:

a) Syngas only from coal
b) Syngas from coal blended with biomass syngas
c) Syngas blended with natural gas
d) Syngas blended with naphtha

The study reveals some important results such as the fuel gas temperature and pressure of feed to the gas turbine are in direct proportion with the power produced in gas turbine. As fuel gas temperature and stream pressure increases, the power produced increases. Optimum value of temperature of fuel gas is taken as 900-1500 ^{o}C. The overall power generated is calculated for different combinations of feed pressures.

Gauging the difficulty in availability and rising prices of petroleum feedstock, the present day approach of using biomass for power generation at large scale is analyzed in chapter 6. Biomass is currently used to generate steam using steam turbine as well as Heat Recovery Steam Generators. We didn't use the conventional inefficient route. We implied biomass generated syngas cleaning methodology and fed this fuel to gas turbine directly. This has served the purpose and gasification as well as power plant efficiency has been improved to an appreciable level. A simulation study has been carried out to arrive at the power output under limiting conditions as well as perform changes in the fuel gas system for the augmentation. The simulation study has been carried out on the simulation software Aspen HYSYS® and the findings show that, the available fuel gas obtained from the biomass can be optimally used for the power generation in the gas turbine. Based on the importance and promising nature of the gasification of biomass, modeling and simulation has been performed for finding the optimum parameters of the process.

Some interesting trends have been obtained, especially with respect to the effect of net heating rate and temperature on the final combustion time. The range of operating conditions used for simulating the model equations is small in the case of the earlier investigators work, but the results obtained using a wide range of operating conditions in the present study show that the final combustion time initially decreases and then increases as the net heating rate or temperature is increased, giving an optimum final combustion time corresponding to the optimum net heat rate or temperature.The simulation study shows that maximum possible power is generated with 79221 NM^3/hr of fuel gas flow bypassing the heater skid which saves 1300 kWh electric power as energy on heating the gas. Maximum possible power generation in each GTG is approximately 145 MW. The gasifier efficiency is enhanced using lumping parameter models for reactions by maintaining inlet temperature below 1400 ^{o}C. This helps for complete conversion of CO and NO_x, which in turn reduces pollution and makes this as a process of clean power production.

A user friendly modular simulation model is developed using popular front end programming language Visual Basic. Data for calculations is provided through back end from MS-SQL. The model is also further embedded into AutoCAD to generate mechanical design parameters. Advantage earned through this embedding is industry scale scale-up facility generated. The present design can now be used at any scale as of requirement of a chemical process plant.

A complete overview of energy analysis, enhancement in present real power plants with design constraints, improvisation in conventional gasifiers, innovative design of horizontal feeder gasifier, newer approach of combined feed usage for reducing single fuel dependency, and large scale efficient system development using non conventional and renewable energy resources are the salient features of the present study. These aspects touch to almost all walks of energy scenario as well as needs of society. An effort is made to provide solutions on all such difficulties converting them into opportunities with viable and rigid suggestions using modern and advanced simulation tools. By virtue of the simulating capacities of such simulation and optimization tools, various results are derived and are presented in this report. These results, in turn, endorse many accomplishments by the present researchers with success in the endeavours towards establishment of innovative, efficient, cleaner, greener, and environmentally friendly energy generation technologies. We look back at it as a step towards sustainable development.

CHAPTER -1

SIMULATION TECHNIQUES AND ENERGY SECURITY

This chapter provides a brief introduction about design, modeling, simulation and optimization tool Aspen HYSYS® from AspenTech, Inc. This is the largest applied simulation tool in the world and many revamping and optimization scenarios are built by extensive use of this simulator. Chapter 1 also provides review and information on energy availability and security as the applied topic of the present study. The collective information emphasizes the immediate need and attention of researchers to provide efficiency enhancement techniques to the world along with newer energy resources and technology as a long term goal. The present researchers have chosen this as the opportunity to work in the energy sector and apply the modern tools for the benefit of masses.

Keywords: design, modeling, simulation, optimization, Aspen HYSYS®, energy availability and security

1.1 INTRODUCTION

The chemical industry has undergone significant changes during the past 25 years due to the increased cost of energy, increasingly stringent environmental regulations, and global competition in product pricing and quality. One of the most important engineering tools for addressing these issues is modeling, simulation and optimization. Modifications in plant design and operating procedures have been implemented to reduce costs and meet constraints, with an emphasis on improving efficiency and increasing profitability. Optimal operating conditions can be implemented via increased automation at the process, plant, and company levels. As the power of computers has increased, the size and complexity of problems that can be solved by optimization techniques have correspondingly expanded.

While designing a chemical product or process, it is important to understand that design problems are open ended and may have many solutions that are attractive and near optimal. Furthermore, no two designers design a complex product or process following exactly the same steps. In fact, to capture the know-how of experienced designers and better understand the design process, cognitive scientists recommend that the designer's steps be tracked so that others can learn to apply them when working on the design of similar products and processes.

Design is the most creative of engineering activities, with many opportunities to invent imaginative new products and processes. It is also the essence of engineering, differentiating an engineer from a scientist. Chemical engineers engaged in product or process development exercise put forth their creativity in formulating experiments and theories to uncover and explain the mechanisms of processing operations, often involving complex reaction kinetics with heat and mass transfer in various flow fields. Chemical engineers engaged in product and process design face different challenges such as: (1) determining the composition of chemical mixtures to provide desired properties, (2) creating complex flowsheets and selecting operating conditions to produce desired products with a high degree of yield and selectivity, little recycle, and low utility costs, and (3) creating configured industrial and consumer products. The creation of product and process designs are rarely straightforward and routine; rather they involve innovative approaches that lead to more profitable products and processes that are environmentally sound, and operationally safe[1].

Formal methods of optimization can be utilized to optimize a superstructure of process units with streams that can be turned on and off using binary (integer) variables. In principle, the *mixed-integer formulation* (involving both continuous and integer variables) of the optimization problem permits the optimizer to select simultaneously the best flowsheet and then optimize it with respect to its continuous variables, such as pressure levels, reflux ratios, residence times, and split fractions. In practice, however, most design problems are not solved using superstructures and mixed-integer optimization algorithms. Rather, heuristics together with simulation and algorithmic methods are utilized to build and analyze *synthesis trees.* Although substructures, such as networks of heat exchangers, can be optimized conveniently using mixed-integer methods, it is impractical, except for simple processes, to attempt the optimization of entire process flowsheets in this manner. Accordingly, this work is restricted to the case of optimization problems involving continuous variables, of either the LP (linear programming) type or the NLP (nonlinear programming) type.

Emphasis is placed in this chapter on the usage of process simulators to carry out the optimization simultaneously with converging the recycle loops and/or decision variables. To do the optimization efficiently, simulators use one of three methods: (1) *successive linear programming* (SLP), (2) *successive quadratic programming* (SQP), and (3) *generalized reduced gradient (*GRG). Emphasis in this chapter is on SQP, used by ASPEN PLUS and HYSYS.

In recent years availability of power in India has both, increased and improved, but demand has consistently outstripped supply. Substantial energy and peak shortages prevailed in the year 2013-‘14. There are also various estimates of 25000 to 35000 MW of power being produced by diesel generation to meet the deficits. Electricity shortage is not the only problem. Its spread is an equally serious issue. In the past, the selection of an energy resource for electricity generation was dominated by finding the least expensive power generating plant. Although such an approach is essential, there is growing concern about other aspects of power generation such as social, environmental and technological benefits and consequences of the energy source selection.

The demand for energy has grown at an average of 3.6% per annum over the past few years. This rapid increase in use of energy has created problems of demand and supply. More than 80,000 villages are yet to be electrified. Around 44% of households do not have access to the electricity. India faces a significant challenge in providing access to adequate, affordable and clean sources of energy, especially cooking fuel to a large section of the population, most of who live in rural areas [2]. On the other hand, the incidence of dependence on firewood for cooking in urban areas has fallen from about 30% to 17.5% between 1993-94 and 2009-10 – a drop of more than 12 percentage points – and the incidence of dependence on kerosene has plunged from 23.2% to 6.5% during the same period – a 72% fall, while the percentage of urban households using LPG has more than doubled from under 30% to 64.5% [3]. Further, as per the NSSO Reports (55th, 61st and 66th Rounds) [4], there has been an increase in biomass fuel use in terms of absolute quantity consumed over the past decade among rural households. This is an area of concern given the considerable health impacts of burning biomass fuels apart from being a hindrance to achieving developmental goals, ensuring a minimum standard of living and provisioning of basic minimum needs. Thus, a transition to cleaner forms of energy in terms of access to electricity and other modern energy forms would have implications not only on energy security, but also with respect to enabling gender equality and bring about greater development and social progress.

1.2 Aspen HYSYS®: A process simulation and optimization tool

HYSYS has been uniquely created with respect to the program architecture, interface design, engineering capabilities, and interactive operation. The integrated steady state and dynamic modeling capabilities, where the same model can be evaluated from either perspective with full sharing of process information, represent a significant advancement in the engineering software industry.

The multi-flowsheet architecture of HYSYS is vital to this overall modeling approach. Although HYSYS has been designed to allow the use of multiple property packages and the creation of prebuilt templates, the greatest advantage of using multiple flowsheets is that they provide an extremely effective way to organize large processes. By breaking flowsheets into smaller components, one can easily isolate any aspect for detailed analysis. HYSYS uses a variety of methods to display process information - individual property views, the PFD, Workbook, Databook, graphical Performance Profiles, and Tabular Summaries. Not only are all of these display types simultaneously available, but through the object-oriented design, every piece of displayed information is automatically updated whenever conditions change. The inherent flexibility of HYSYS allows for the use of third party design options and custom-built unit operations. These can be linked to HYSYS through OLE Extensibility [6].

HYSYS offers a high degree of flexibility because there are multiple ways to accomplish specific tasks. This flexibility combined with a consistent and logical approach to how these capabilities are delivered makes HYSYS an extremely versatile process simulation tool. The usability of HYSYS is attributed to the following four key aspects of its design:

- Event Driven operation
- Modular Operations
- Multi-flowsheet Architecture
- Object Oriented Design

Each key aspect is elaborated below.

1.2.1 Event Driven: This concept combines the power of interactive simulation with instantaneous access to information. Interactive simulation means the information is processed as it is supplied and calculations are performed automatically. Also, it is restricted to the program location where the information is supplied.

1.2.2 Modular Operations: Modular Operations are combined with the Non-Sequential solution algorithm. Not only is information processed as it is supplied, but the results of any calculation are automatically produced throughout the flowsheet, both forwards and backwards.

1.2.3 Multi-flowsheet Architecture: Multi-flowsheet architecture can be used to create any number of flowsheets within a simulation and to easily associate a fluid package with a defined group of unit operations.

1.2.4 Object Oriented Design: The separation of interface elements (how the information appears) from the underlying engineering code means the same information appears simultaneously in a variety of locations. Each display is tied to the same process variable, so if the information changes, it automatically updates in every location. Also, if a variable is specified, then it is shown as a specification in every location. This means the specification can be changed wherever it appears and is not restricted to a single location for making changes [6].

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1.3 THE ENERGY SCENARIO

Figures 1.1 and 1.2 informs about the total energy supply of world in present years along with its stand compared to 1973 in terms of Mtoe (Million Tonnes of Oil Equivalent) for Total Primary Energy Supply (TPES). Figures 1.4 and 1.5 indicate the consumption pattern during the same time duration. The figures indicate that the supply had not been completely used for energy production due to various limitations including supply chain management, inefficient technologies and unaffordable prices of energy. Figures 1.3 and 1.6 provide the supply and consumption data of fuels for Organization for Economic Cooperation and Development (OECD) countries. Data for primary sources and other fuels (which include geothermal, solar, wind, heat, etc.) are provided. *Key World Energy Statistics 2013*, OECD Publishing, International Energy Agency (IEA) [7] has elaborated on the supply and consumption pattern along with fuel types and regions.

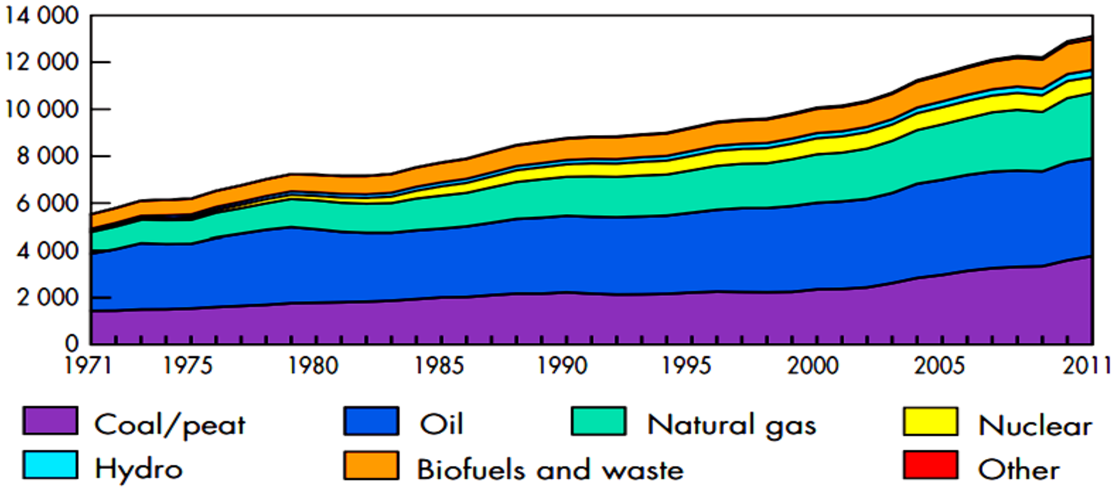


Fig. 1.1: World total primary energy supply from 1971 to 2011 by fuel (Mtoe)

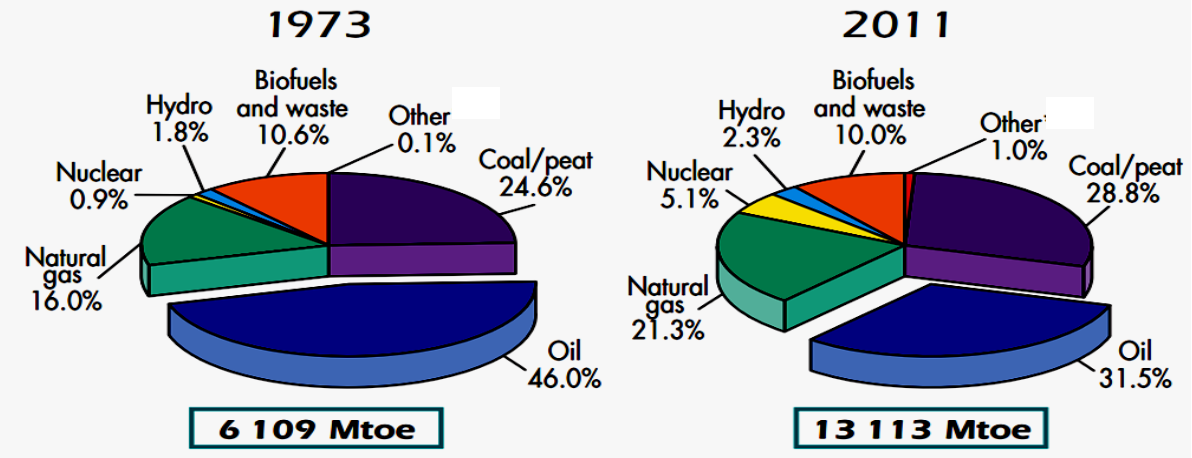


Fig. 1.2: 1973 and 2011 fuel shares of TPES

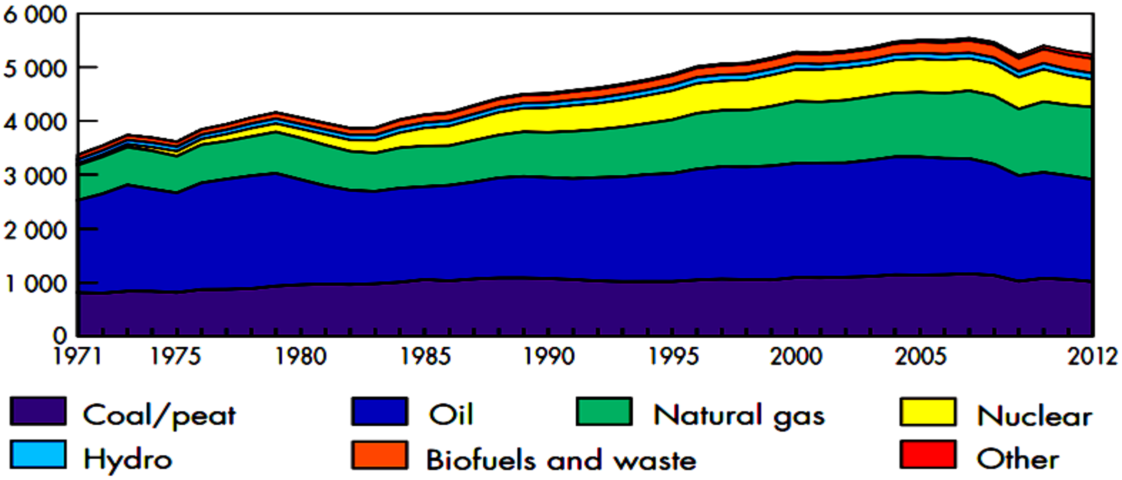


Fig. 1.3: OECD total primary energy supply from 1971 to 2012 by fuel (Mtoe)

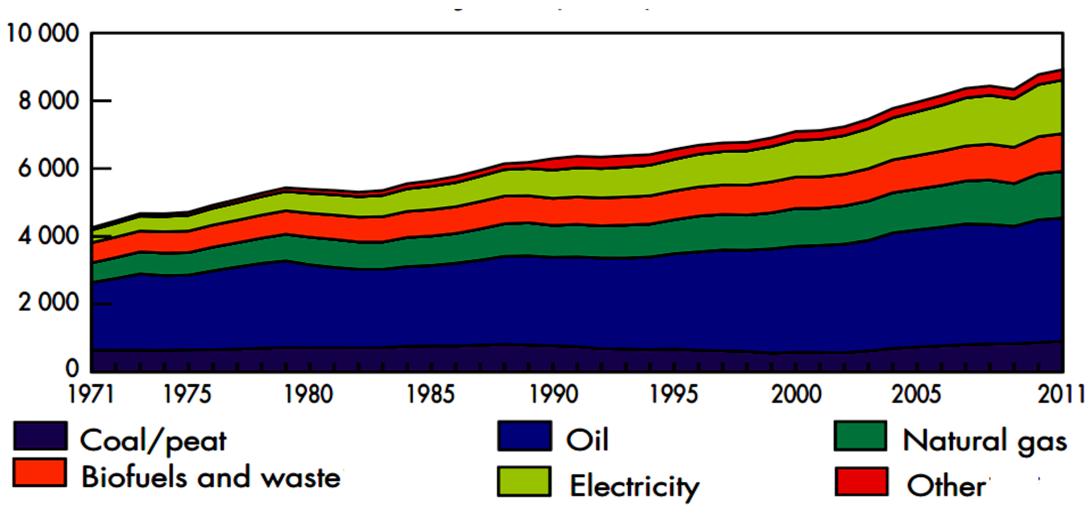


Fig. 1.4: World total final consumption from 1971 to 2011by fuel (Mtoe)

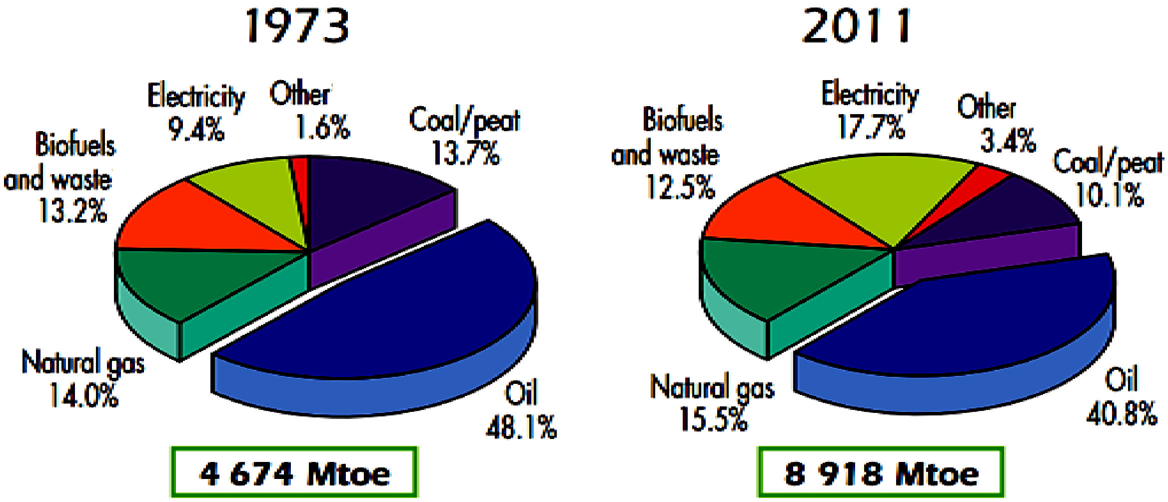


Fig. 1.5: 1973 and 2011 fuel shares of total final consumption

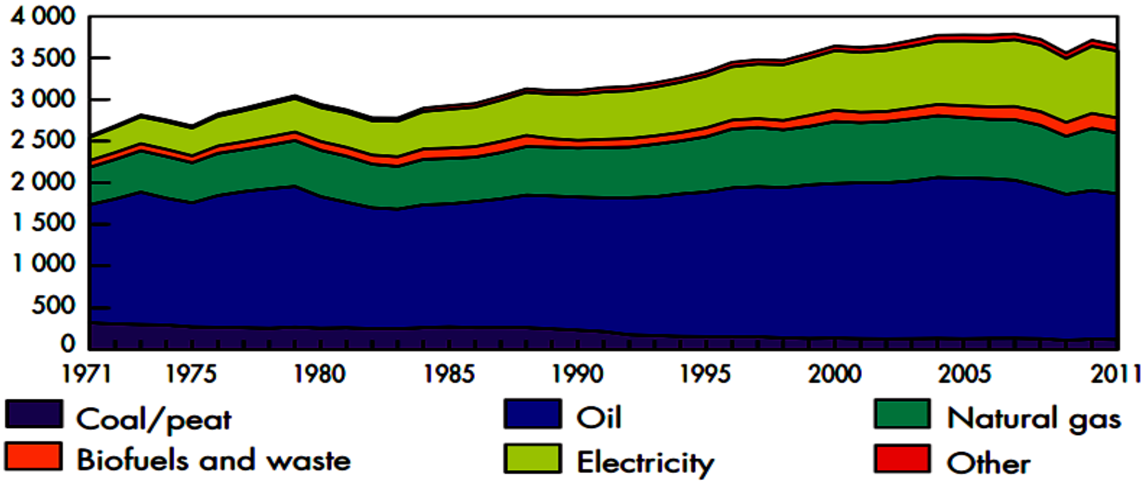


Fig. 1.6: OECD total final consumption from 1971 to 2011 by fuel (Mtoe)

Above data emphasizes that, along with newer energy resources, efficient tools and technologies are essential to utilize the available energy resources at the best and at affordable prices.

Figure 1.7 gives the comparison of India with other regions of the world with regards to Total Primary Energy Supply (TPES) which has been normalized with respect to GDP and population for the year 2013[8].

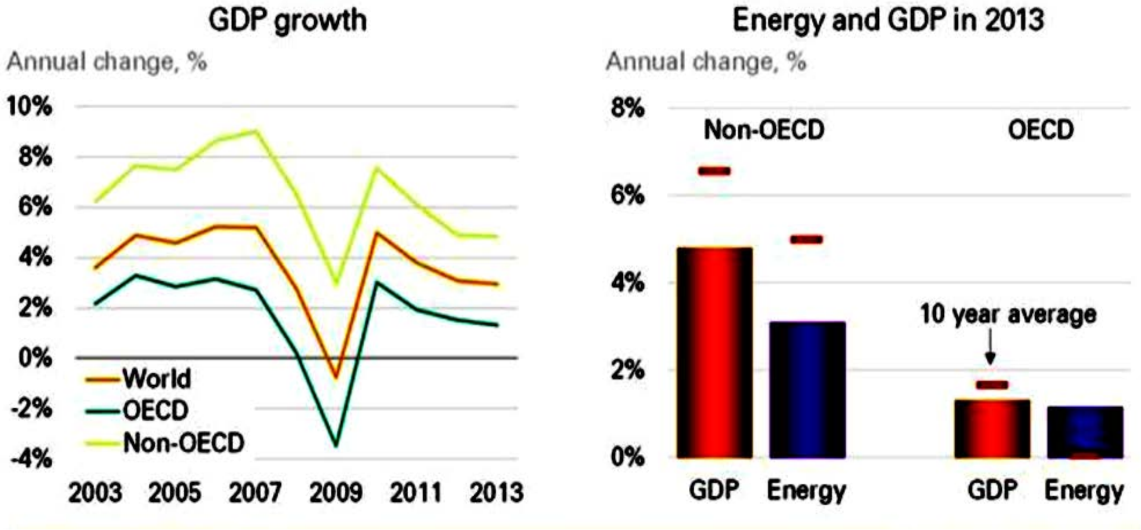


Fig. 1.7: World GDP growth and energy requirement rise

From figure 1.8, it can be seen that per capita consumption of energy in India is one of the lowest in the world. India consumed 540 kgoe (kilogram of oil equivalent) in 2013 compared to 1803 kgoe by the world average, 4560 kgoe by OECD countries, and 1600 kgoe by China. India's energy use efficiency for generating Gross Domestic Product (GDP) in Purchasing Power Parity is better than many countries and even compared to the world average. It is expected that with a growth rate of 9%, Total Primary Energy Supply (TPES) requirement for India in 2021-22 will be around 1192 Mtoe (Million Tonnes of Oil Equivalent) which will further increase to around 2043 Mtoe by the year 2031-32.

The electricity consumption per capita for India is just 566 kWh and is far below most other countries or regions in the world. Even though 85% of villages are considered electrified, around 57% of the rural households and 12% of urban households, i.e. 84 million households in the country, do not have access to electricity. Electricity consumption in India is expected to rise to around 2280 BkWh by 2021-22 and around 4500 BkWh by 2031-32[9, 10].

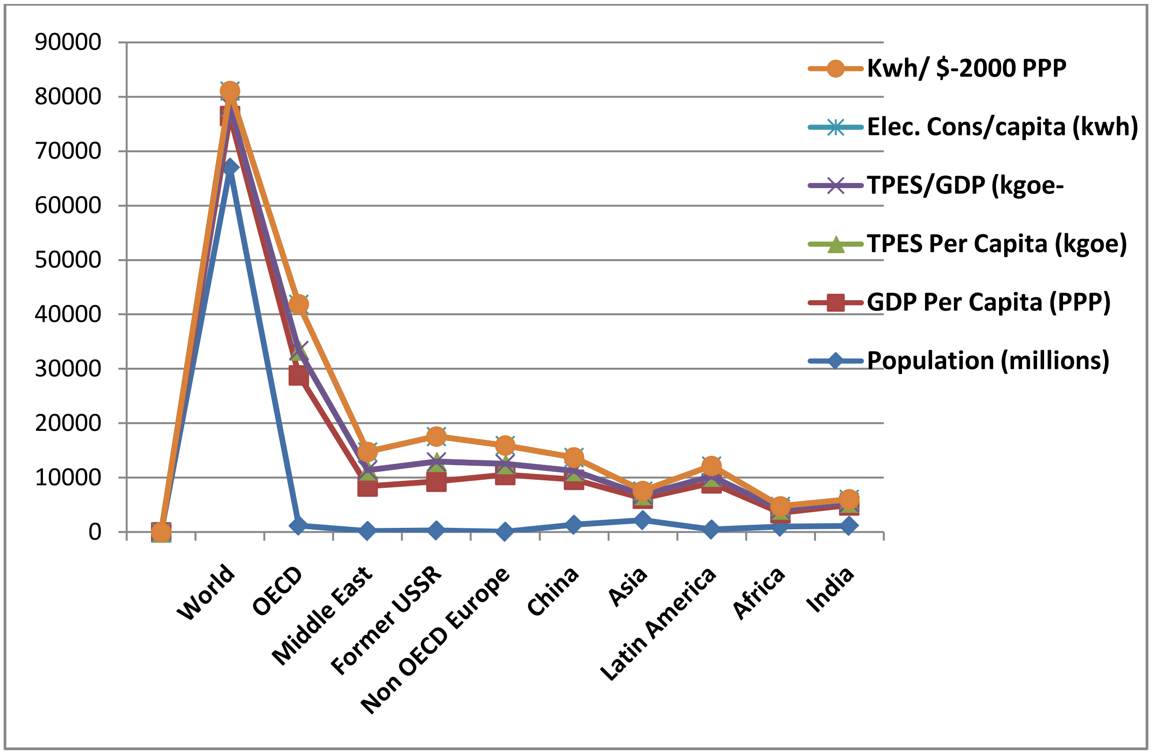


Fig. 1.8: Energy scenario for world and India

1.4 PRODUCTION OF PRIMARY SOURCES OF CONVENTIONAL ENERGY IN INDIA

1.4.1Production of coal, lignite, crude petroleum, natural gas, and electricity

Production of crude petroleum increased from 6.82 MTs during 1970-71 to 38.09 MTs during 2011-12, a CAGR of about 4.18%. The CAGRs for natural gas and electricity were 8.67% and 4.33%, respectively. Natural gas has experienced the highest CAGR among all the conventional sources of energy. The production of energy in peta Joules by primary sources shows that Coal and Lignite were the major sources of energy, accounting for about 50.23% of the total production during 2011-12. Electricity was second (31.48%), while Natural Gas

(9.78%) was third. The Compound Annual Growth Rate of production of energy in India by primary sources from 1970-71 to 2011-12 is shown in figure 1.9.

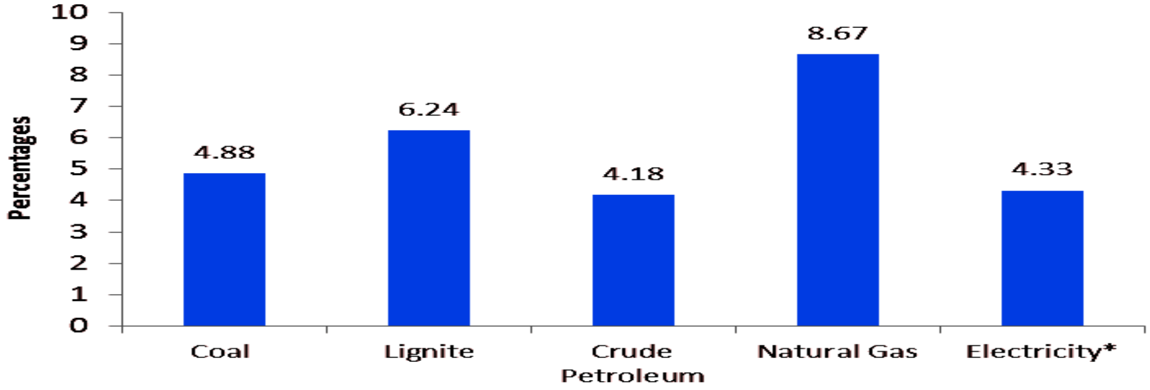


Fig. 1.9: Annual growth of production of energy in India

Table 1.1 shows total power generation capacity of India till March 2013. The data underlines need of immediate attention towards newer technological adaptations for meeting growing demand of electricity.

Table 1.1: All India region wise installed capacity (MW) of Power utilities [11]

Sl. No.	REGION	THERMAL				Nuclear	HYDRO	R.E.S.	TOTAL
		COAL	GAS	DSL	TOTAL				
1	Northern	32413.50	4781.26	12.99	37207.75	1620.00	15467.75	5589.25	59884.75
2	Western	49257.01	8988.31	17.48	58262.80	1840.00	7447.50	8986.93	76537.23
3	Southern	25032.50	4962.78	939.32	30934.60	1320.00	11353.03	12251.85	55859.48
4	Eastern	23457.88	190.00	17.20	23665.08	0.00	3981.12	454.91	28101.11
5	N. Eastern	60.00	1187.50	142.74	1390.24	0.00	1242.00	252.68	2884.92
6	Islands	0.00	0.00	70.02	70.02	0.00	0.00	6.10	76.12
7	**All India**	**130220.89**	**20109.85**	**1199.75**	**151530.49**	**4780.00**	**39491.40**	**27541.71**	**223343.60**

Renewable Energy Sources (RES) includes Small Hydro Project (SHP), Biomass Power (BP), Urban & Industrial waste Power(U&I), Wind Energy and Solar Power.

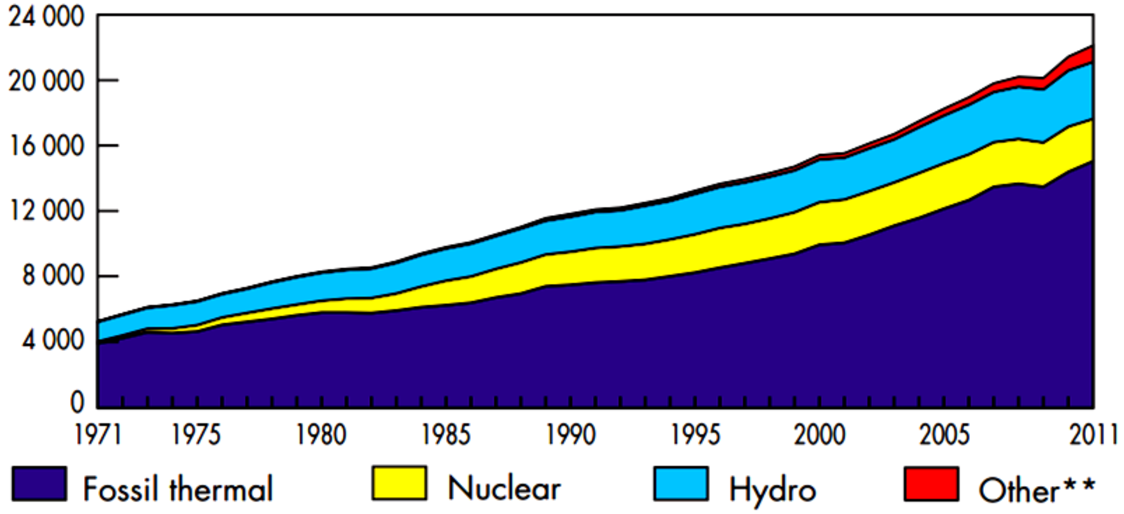
For more meaningful comparison in the trends and patterns of growth of different energy resources, it is desirable to convert all the resources to their energy equivalents by applying appropriate conversion factors and express them in energy units (Joules/ peta Joules/ terra Joules). The total production of energy from conventional sources increased from 17857 peta Joules during 2010-11 to 18734 peta joules during 2011-12, showing an increase of 4.91% [10]. The year wise details of electricity generation using conventional resources are provided in table 1.2.

Table 1.2: Production of primary sources of conventional energy in India [10]

Year	Coal (mtone)	Lignite (mtone)	Crude oil (mtone)	Natural Gas (Billion Cubic Metres)	Electricity (GWh)
1970-71	72.95	3.39	18.38	0.65	43,724
1975-76	99.68	3.03	22.28	1.13	60,246
1980-81	114.01	5.10	25.84	1.52	82,367
1985-86	154.30	7.68	42.91	4.95	123,099
1990-91	213.86	14.07	51.77	12.77	190,357
1995-96	273.42	22.15	58.74	18.09	277,029
2000-01	313.70	24.25	103.44	27.86	316,600
2005-06	407.04	30.34	130.11	31.03	411,887
2006-07	430.83	30.80	146.55	30.79	455,748
2007-08	457.08	34.66	156.10	31.48	510,899
2008-09	492.76	31.79	160.77	31.75	562,888
2009-10	532.04	34.43	192.77	46.51	620,251
2010-11	532.69	37.69	206.15	51.25	684,324
2011-12	539.94	41.88	211.42	46.48	755,847
Growth rate of 2011-12 over 2010-11(%)	**0.60**	**11.14**	**2.56**	**-9.30**	**10.45**
CAGR 1970-71 to 2011-12(%)	**4.86**	**6.17**	**5.99**	**10.71**	**7.02**

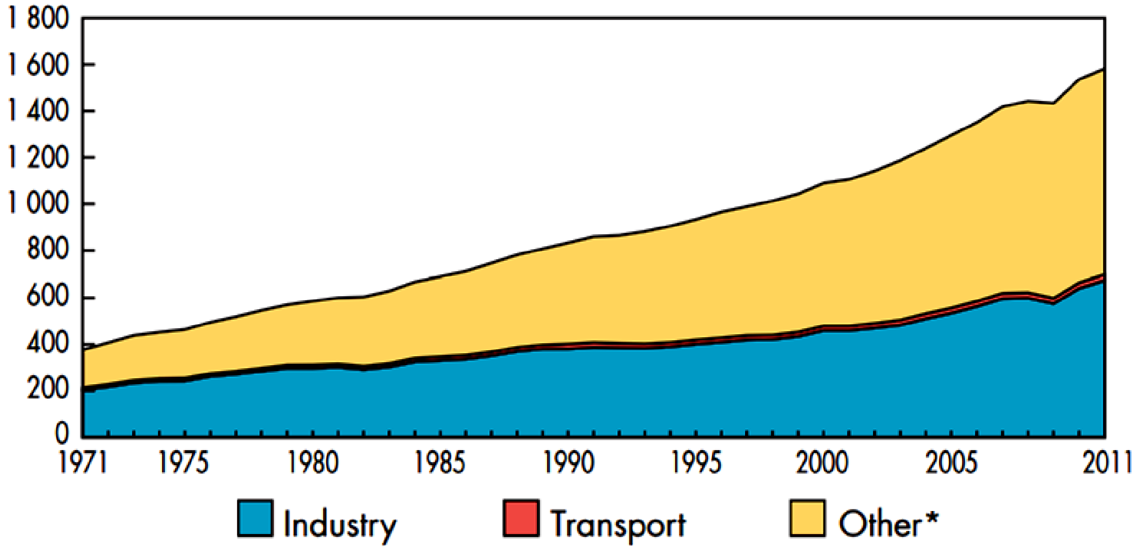
1.5 Electricity Generating Capacity in the world

Figures 1.10 and 1.11 illustrates the world energy generation in TWh and final consumption by sectors in Mtoe. The increasing component of others, which includes geothermal, solar, wind, biofuels and waste, and heat, is quite remarkable and shows the direction of future energy resources for electricity generation [7].



***Other includes geothermal, solar, wind, biofuels and waste, and heat.*

Fig 1.10 World electricity generation from 1971 to 2011 by fuel (TWh)



**Other includes agriculture, commercial and public services, residential, and non-specified other.*

Fig 1.11 Electricity: total final consumption from 1971 to 2011 by sector (Mtoe)

1.6 Electricity Generating Capacity in India

As illustrated by figure 1.12, the total installed capacity for electricity generation in the country has increased from 16,271 MW as on 31.03.1971 to 2, 36,387 MW as on 31.03.2012, registering a compound annual growth rate (CAGR) of 6.58%

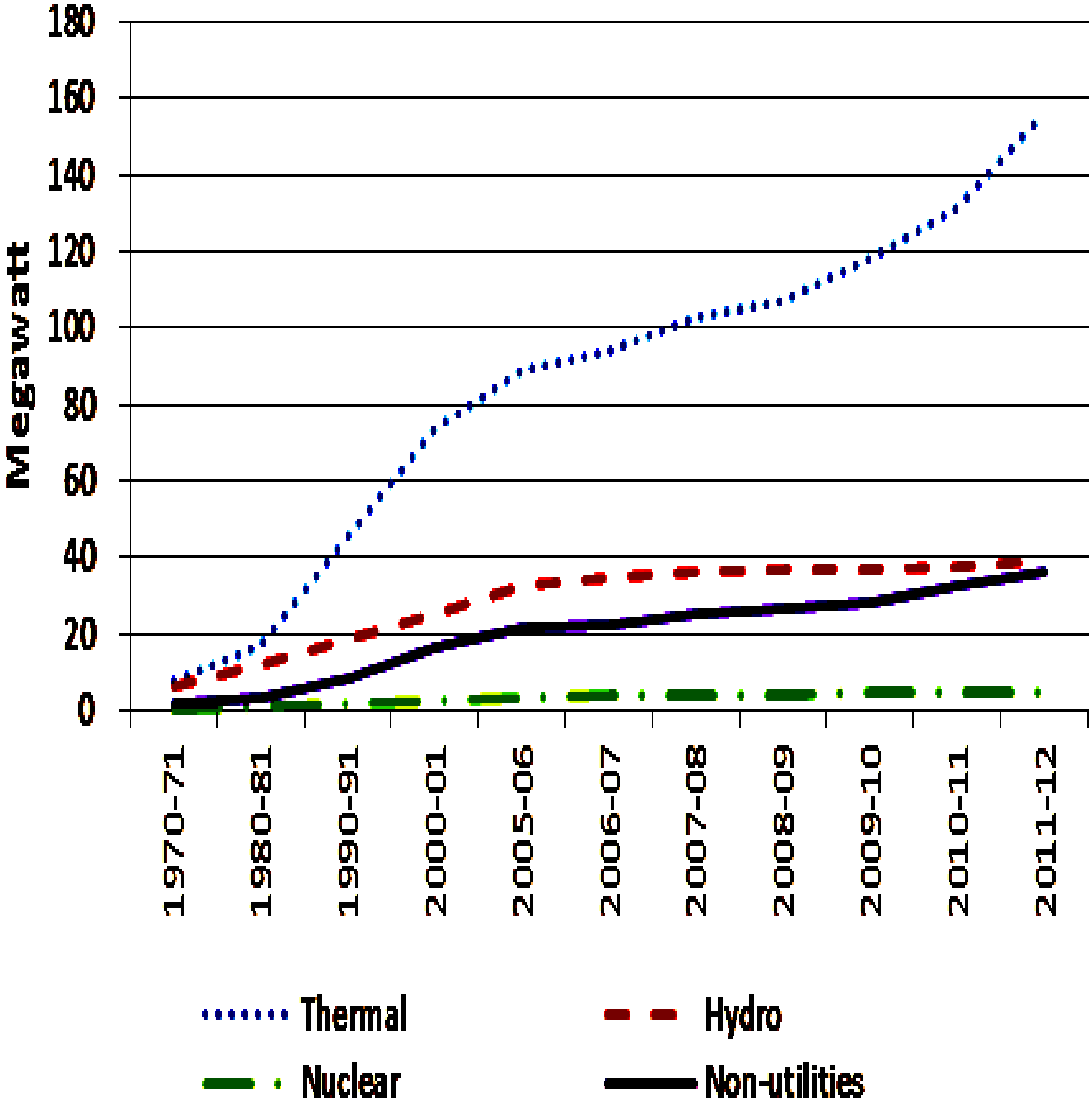


Fig 1.12: Electricity generating capacity in India

The highest CAGR (7.36%) was in case of Thermal utilities followed by Nuclear (5.96%) and Hydro (4.4%). The CAGR of installed generating capacity with various power generation methods are shown in figure 1.13 [10].

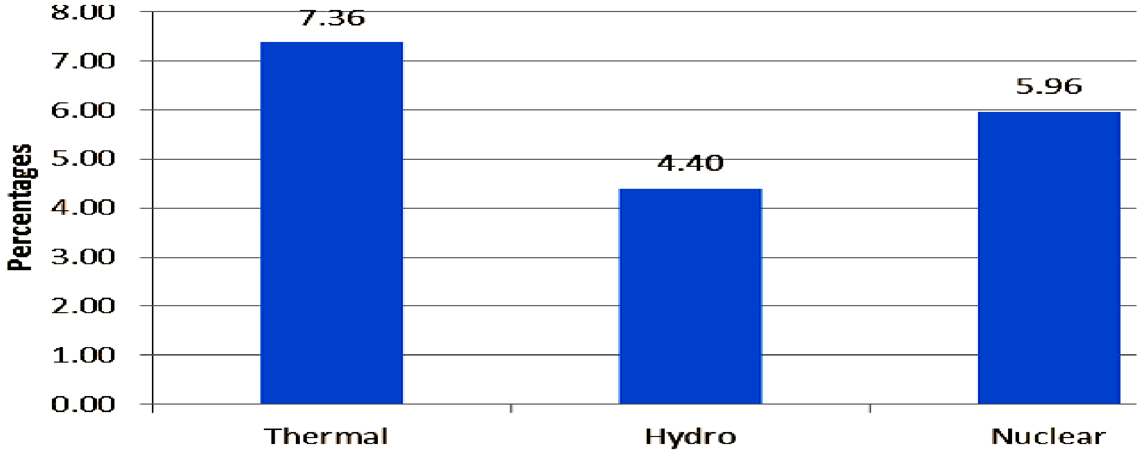


Fig 1.13: Annual growth of electricity generating capacity [10]

1.7 Power Generation

Category wise Gross Electricity Generation performance for India till March 2013 is shown in table 1.3. The desired production of power could not be achieved due to various reasons such as non availability of good quality fuel as well as capital and human resources along with non implementation of advanced technologies.

Table 1.3: The category-wise details of electricity generation in the country

Category	Programmed (BU)	Actual Generation (BU)	% of program	Actual Generation (BU)	Growth
Thermal	71.98	68.49	95.16	66.14	-3.55
Nuclear	3.46	2.71	78.2	2.86	5.33
Hydro	8.00	8.68	108.51	8.53	1.72
Total	83.44	79.88	95.73	77.53	-2.94

1.8 Availability of fuel supply in India

1.8.1 Availability of coal and lignite

The total availability of raw coal in India during 2011-12 stood at 638.84 MTs and that of lignite at 41.89 MTs. The availability of coal in the year 2011-12 increased by 8.30% compared to 2010-11, the availability of lignite also increased by 11.15% during the same period.

1.8.2 Availability of Natural Gas

The availability of natural gas has steadily increased from a mere 17.86 BCMs during 1970-71 to 150.87 BCMs during 2011-12, registering a CAGR of 5.21%. Most of this increase in the indigenous production is due to discovery of new reserves.

1.8.3 Availability of Electricity

Without taking into account the transmission and distribution losses, the total availability is equal to the total generation, and this figure increased from 53,031 GWh during 1970-71 to 8,11,506 GWh during 2011-12, registering a CAGR of 6.71% over the period.

1.8.4 Availability of Crude Oil and Petroleum Products

The availability of crude oil in the country increased from 18.51MTs during 1970-71 to 106.52 MTs during 2000-01 and then to 209.82 MTs during 2011-12. During this period crude oil production increased from 6.82 MTs to 38.09 MTs and the net import increased from 11.68 MTs to 171.73 MTs. There was 4.24% increase in availability of crude oil during 2011-12 over 2010-11.

The availability of fuel sources discussed above is illustrated in figure 1.14.

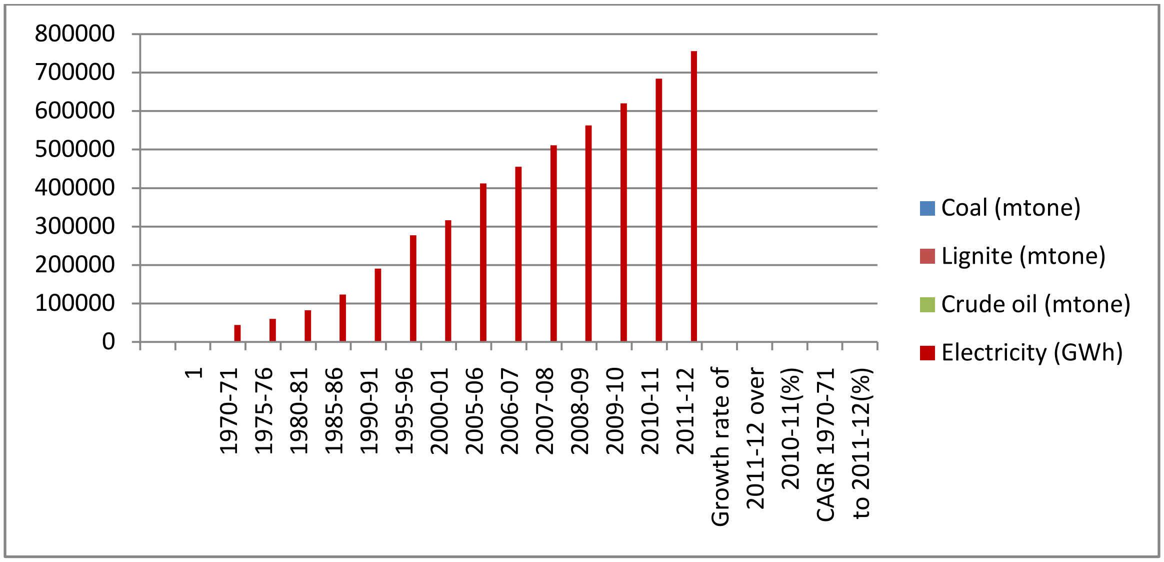


Fig 1.14: Availability of primary sources of conventional energy in India

1.9 NON-RENEWABLE ENERGY

Strategies to meet India’s energy requirement are constrained by country’s energy resources and import possibilities. Unfortunately, India is not well endowed with natural energy resources. Reserves of oil, gas and Uranium are meager though India has large reserves of thorium. While coals abundant, it is regionally concentrated and is of low calorie and high ash content, though it has the advantage of low sulfur content.

Non-renewable energy sources as coal, petroleum oil, natural gas and nuclear oil and their availability are discussed below [10].

1.9.1 Coal: It is the most important and abundant fossil fuel in India. It accounts for 55% of the country's energy need. The country’s industrial heritage has been built upon indigenous coal. Commercial primary energy consumption in India has grown by about 70% in the last four decades. Considering the limited reserve potentiality of petroleum and natural gas, eco-conservation restriction on hydro projects and geo-political perception of nuclear power, coal will continue to occupy centre-stage of India’s energy.

At present, the total cost of power generation using domestic coal is ₹ 2.1 per kWh. But with imported coal, the cost shoots up to ₹ 3.6 per kWh, due to high international coal prices, port handling charges, and customs duty. Coal based generation remains constrained in India due to materialization of the requirement of coal. A challenge to the power industry is to maintain capacity utilization at high levels. Further, The Directorate General of Hydrocarbons has estimated the country's resource base for Coal Bed Methane (CBM) to be between 1400 BCM (1260 Mtoe) and 2600 BCM (2340 Mtoe).To give impetus to exploration and production, the government has formulated the CBM policy [10].

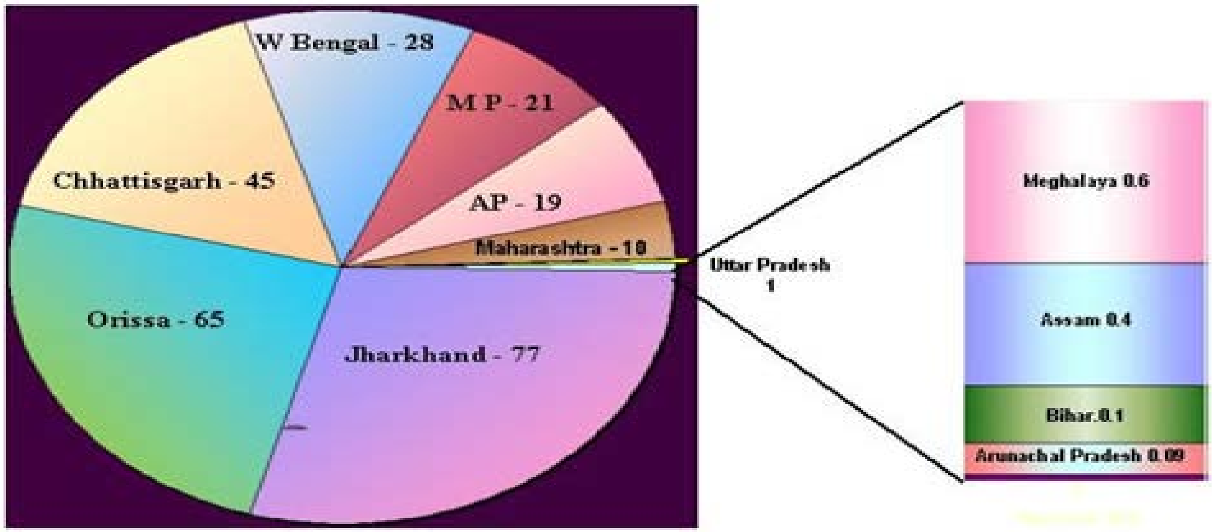


Fig 1.15: State wise coal resources in India (in billion tonnes)

1.9.2 Petroleum Oil: India has total reserves (proved and indicated) of 1201 million metric tonnes of crude oil. Crude oil production during 2009-10 at 33.69 million metric tonnes was 0.55% higher than the 33.51 million metric tonnes produced during 2008-09.

1.9.3 Natural gas: India has total reserves (proved and indicated) of 437 billion cubic meters of natural gas as of 1st April 2010**.** Gross Production of Natural Gas in the country at 47.51 billion cubic meters during 2009-10 was 44.63% higher than the production of 32.85 billion cubic meters during 2008-09. The total installed capacity of gas fired plants as of February 2011 stood at 17706 MW.

The flaring of Natural Gas in 2009-10 at 2.09% of gross production is lower than the 3.29% in 2008-09.

The cost of power obtained by using natural gas varies from ₹ 2.90 to ₹ 4.60 per kWh and power obtained through natural gas is mainly used as peaking power. India Vision 2020 has estimated the demand for gas to be between 65 and 71 Billion Cubic Meters (BCM) for the year 2020. IRADe-PWC has projected demand of natural gas and natural gas equivalent of Naphtha at 243 BCM under the business as usual scenario and 405.7 BCM under a High Output Growth scenario for the year 2030 [11].

1.9.4 Nuclear energy: Nuclear power is the fourth-largest source of electricity in India after thermal, hydroelectric and renewable sources of electricity. As of 2010, India has 20 nuclear reactors in operation in six nuclear power plants, generating 4,780 MW while 5 other plants are under construction and are expected to generate an additional 2,720 MW. The nuclear power parks are planned at Kudankulam in Tamil Nadu, Jaitpur in Maharashtra, Mithi Verdi in Gujarat, Haripur in West Bengal and Kovvada in Andhra Pradesh [12].

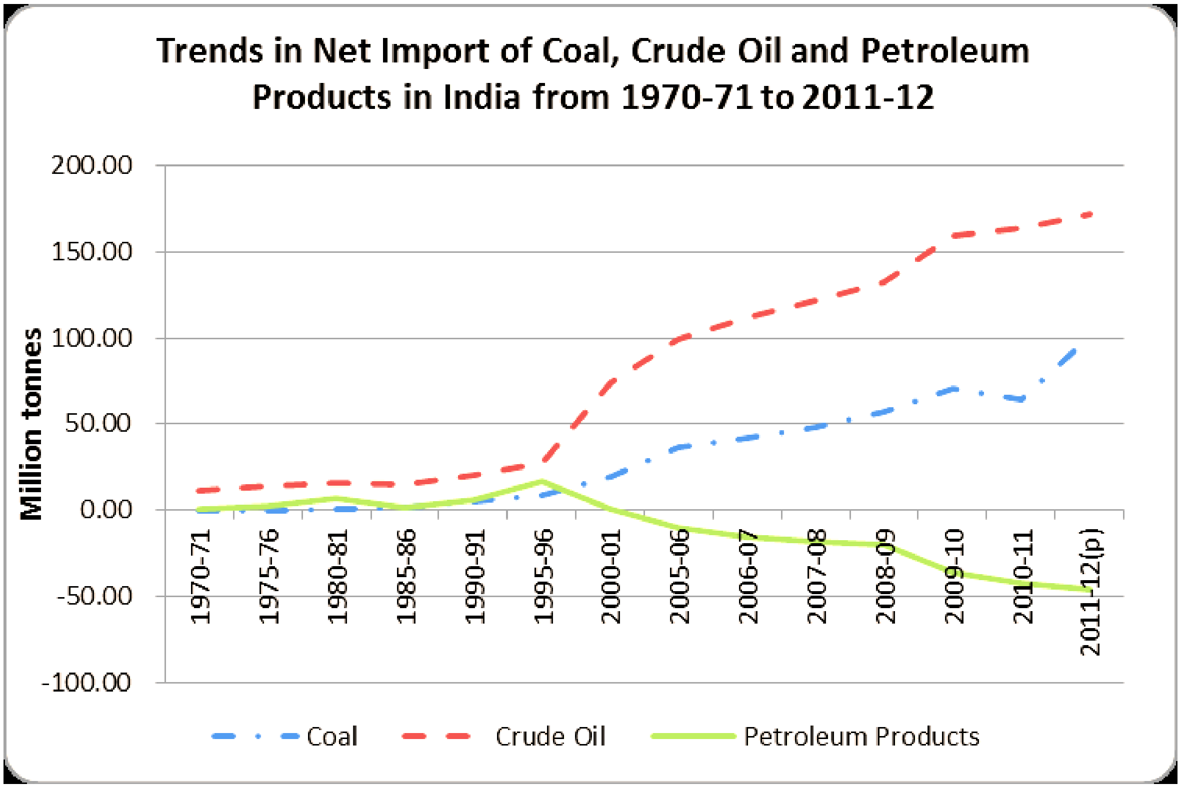


Fig 1.16: Import of non- renewable energy in India [12]

1.10 RENEWABLE ENERGY

India has been making continuous progress in conventional as well as renewable power generation. The trajectory of growth of installed capacity since 2002 (start of the 10th five year Plan), 2007 (start of 11th Plan), and as of November 30, 2010 is given in table 5 below. It is observed from the table that renewable grid capacity has increased more than 5 times in a span of 8 years and this compares favorably with the EU and far exceeds that of the US [13].

Table 1.4: Growth of installed capacity of power resources in India

Time period	Thermal (%) (MW)	Hydro (%) (>25MW) MW	Nuclear (%) (MW)	Renewable Power (%) (MW)
1.4.2002	70.85% 74429	25% 26269	2.59% 2720	1.55% 1628

1.4.2007	64.06% 87015	25.51% 34654	2.87% 3900	7.55% 10258
31.9.2010	63.95% 106518	22.41% 37328	2.7% 4560	10.90% 18,155

Wind, bio, hydro and solar energy resources and their installed capacities in India are discussed below.

1.10.1 Wind Power

India, with a total of 19565 MW as of June 30, 2013; has the fifth largest installed capacity of wind power in the world. She is just behind China, USA, Germany and Spain. For comparison, as of June 2013, Germany had an installed capacity of (32422 MW) for wind power [14].

1.10.2 Hydro Power

Hydro projects in India, which are under 25 MW in capacity, are classified as “small hydropower” and considered as a “renewable” energy source. The total cumulative installed capacity for grid connected small hydropower plants and off-grid micro hydro plants (up to 100 kWh) in India up to June 30, 2013 was 3,686 MW [15].

1.10.3 Bio Energy

Bio energy can be categorized into biomass, bio fuels and biogas. In India, a total of 4449 MW has been installed under bio energy, both in grid connected and off-grid capacities. Table 1.5 gives the details of the installations under the different categories of bio energy up to June 2013.

Table 1.5: Installations under bio energy in India (as on June 30, 2013)

Bio-energy Type	**Capacity installed (MW)**
Biomass Power	1,265

Bagasse Cogeneration	2,337
Waste to Power (urban)	212
Biomass gasifiers (rural)	17
Biomass gasifiers (industrial)	143
Biomass (non-bagasse) cogeneration	475
Total	**4,449**

1.10.4 Solar energy

Grid connected solar power, until the end of 2010, when the installed capacity was still less than 50 MW, had played a relatively insignificant role as compared to other renewable sources of energy in India, such as wind. Since then, however, the solar power industry has grown rapidly. Installed capacity for solar power reached 1.2 GW by the end of 2012 and more than 1.9 GW by the end of July 2013. Grid connected photovoltaic (PV) contributed around 1850 MW to this capacity and off grid photovoltaic amounted to 130 MW. Germany, by comparison, had an installed capacity of 34558 MW by July 2013.

Gujarat was the first to release a state specific solar policy back in 2009. In 2010, the MNRE launched the Jawaharlal Nehru National Solar Mission (NSM) with an aim to add 20GW of solar installations in India by 2022. Following the launch of the NSM, several states such as Karnataka, Gujarat, Rajasthan, Madhya Pradesh and Uttar Pradesh published state specific solar policies, driven by RPOs. The growth in installations since 2010 can primarily be attributed to allocations under the NSM, Gujarat Solar Policy, Karnataka Solar Policy and direct allocations by states such as Madhya Pradesh and Maharashtra. Details about the states policies are given in the section ‘New Policy Developments’ [16].

Renewable energy installed capacity at a glance:

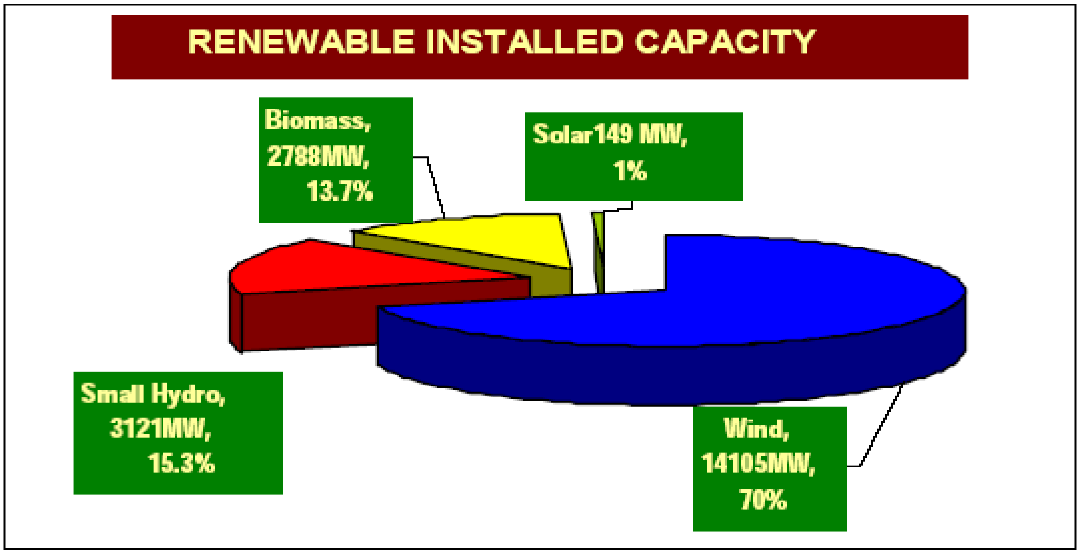


Fig. 1.6: Renewable energy installed capacity in India as on July 2013

1.11 ENERGY and ENVIRONMENT

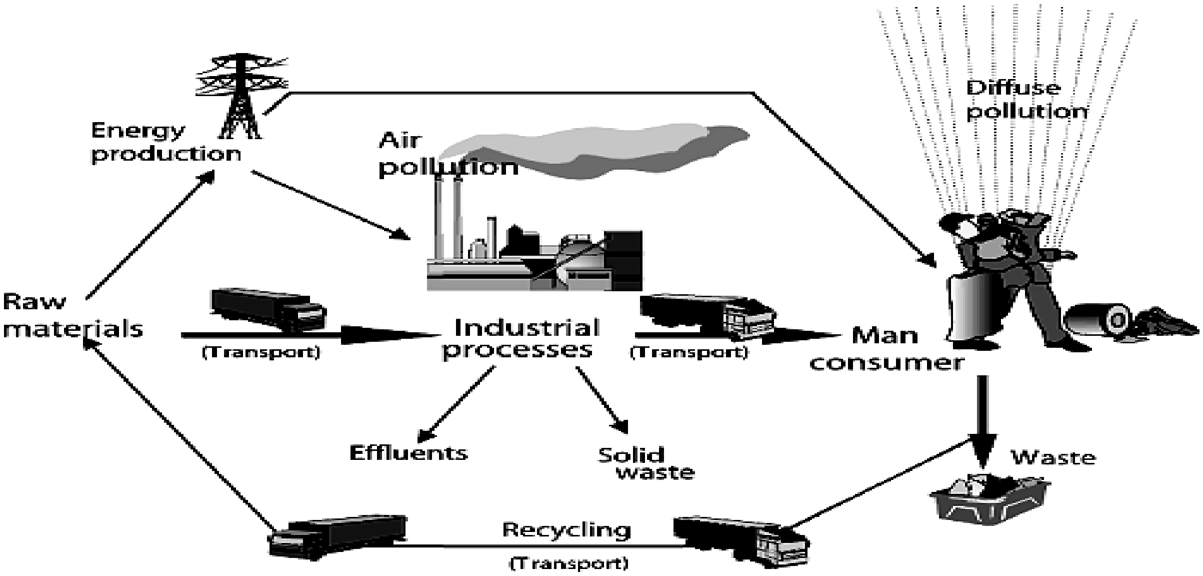


Fig. 1.6: Correlation between pollution due to energy resources

The usage of energy resources in industry leads to environmental damages by polluting the atmosphere. Few of examples of air pollution are sulphur dioxide (SO_2), nitrous oxide (NO_X) and carbon monoxide (CO) emissions from boilers and furnaces, chloro-fluro carbons (CFC) emissions from refrigerants use, etc. In chemical and fertilizers industries, toxic gases are released. Cement plants and power plants spew out particulate matter. Typical inputs, outputs, and emissions for a typical industrial process are shown in figure 1.6.

1.11.1 Future Effects

Even the minimum predicted shifts in climate for the 21st century are likely to be significant and disruptive. Predictions of future climatic changes are wide-ranging. The global temperature may climb from 1.4 to 5.8 ^{o}C; the sea level may rise from 9 to 88 cm. Thus, increases in sea level this century are expected to range from significant to catastrophic. This uncertainty reflects the complexity, interrelatedness, and sensitivity of the natural systems that make up the climate.

1.11.2 Climatic Change

Human activities, particularly the combustion of fossil fuels, have made the blanket of greenhouse gases (water vapour, carbon dioxide, methane, ozone etc.) around the earth thicker. The resulting increase in global temperature is altering the complex web of systems that allow life to thrive on earth such as rainfall, wind patterns, ocean currents and distribution of plant and animal species [17].

1.12 ENERGY CHALLENGES IN INDIA [18-21]

1.12.1 A Reform and restructuring of the energy sector to develop globally competitive, efficient and environmentally compatible operations.

In the pre-reform period, the commercial energy sector was totally regulated by the government. The economic reform and liberalization, in the post 90’s, has gradually welcomed private sector participation in the coal, oil, gas, and electricity sectors in India.

1.12.2 Comprehensive integrated energy planning taking into account the role of hydrocarbons.

Since the energy sector in India is handled by several ministries, there is a need for coordination and integration among them. Reform in the power sector, for example, is suffering from the lack of progress in coal reforms while coal movement suffers from the lack of tariff rationalization in the railways.

Very recently, on August 25, 2014; the honourable Supreme Court of India cancelled all the coal block allocations from 1993 to 2010. There is an immediate need to draft proper policy and framework for exploration of natural resources in India.

1.12.3 Adoption of clean coal technologies and utilization of lower-cost imported coal for coastal power plants.

The Indian power sector is facing challenges and despite significant growth in generation over the years, it has been suffering from shortage and supply constraints. According to Central Electricity Authority (CEA) estimates, the demand for power is expected to double in the next 10-12 years.

1.12.4 Enhancement of strategic oil reserve through accelerated exploration and increased domestic oil supply.

One of the landmarks in liberalization in the petroleum sector is the encouragement of participation of foreign and Indian companies in the exploration and development activities to supplement the efforts of national oil companies. New Exploration Licensing Policy has been put into operation through NELP-I, II and III production sharing contracts and NELP-IV is expected soon.

1.12.5 Achieving 90 percent self-sufficiency of middle distillates with appropriate mix from national oil companies, private Indian players and foreign companies.

In line with international trends, it is estimated that the share of middle distillates, which constitutes a large part of the total demand, would further increase from 59 to 64.6 percent by 2025.

1.12.6 Conditional marketing rights for transportation fuels to companies who invest in exploration and production, refining, pipelines or terminals.

As the objective of dismantling of the Administered Price Mechanism (APM) is to remove the existing controls and usher in a free market, this should be done at the earliest to encourage internal competition.

1.12.7 Operational flexibility to refineries in crude sourcing and risk management through hedging.

The Government should allow every refinery the flexibility to source its own crude, as well as the ability to manage the business risk by using commodity hedges and other risk management techniques. Indian refinery companies should explore the possibility of investing in crude production assets overseas. This would help Indian companies tie up secured crude supplies and also enable them to become strong, integrated, globally competitive entities.

CONCLUSIONS

Energy is vital for development and this means that if India is to move to a higher growth trajectory than is now feasible, it must ensure the reliable availability of energy. The present energy scenario in India is not satisfactory. The power supply position prevailing in the country is characterized by persistent shortages and unreliability and also high prices for industrial consumers. There is also concern about the position regarding petroleum products. India depends to the extent of 70-80percent on imported oil, and this naturally raises issues about energy security.

India needs to realize the vast potential of renewable energy and need to step up effort for attaining the goal of "20 1120 20" by 2020 i.e. 20% reduction in GHG, 11% reduction in consumption of energy by bringing about attitudinal changes, 20% share of renewable energy and 20% conservation of energy from the year 2011 till 2020. These targets are attainable and not only provide cleaner energy but also open a new field for providing employment opportunities to millions of people who are unemployed or disguised employment. This momentum then needs to be maintained so that India attains a target of having70% renewable energy use by 2050.

Energy is central to achieving the interrelated economic, social, and environmental aims of sustainable human development. But if India is to realize this important goal, the kinds of energy India produces and the ways it uses them will have to change. Otherwise, environmental damage will accelerate, inequity will increase, and economic growth will be jeopardized. All energy Sources are having advantages as well as certain disadvantages. As resources are not an end in themselves, and their attractiveness must be seen in the context of societies' energy service needs, of the technologies that convert resources into energy services, and of the economics associated with their use. These analyses have shown that India will have to plan for the fulfillment of its energy needs based on a judicious mix of the natural resources endowed to it, keeping sustainable development in focus and having a minimum carbon foot print. Developed countries of the world also need to understand that climate change is a phenomenon which has no boundaries and the world is facing this threat because of skewed policies followed by them and they are also duty bound to help India attain the goal of achieving energy security for its population by the transfer of clean [energy] technology and by making available appropriate funding mechanisms.

India, with its vast population and limited natural resources for meeting its energy requirements, needs to maintain its momentum of growth and this can be made possible only with a clear strategy for use of best possible energy options available. India needs to have a long term strategy for meeting its energy needs by 2050 and a short term goal of 2020 which can be small steps towards attaining energy security by 2050. The broad vision behind energy policy must be to meet energy demands reliably with energy which is clean and affordable and this must be done in an environmentally sustainable manner using different fuels and forms of energy, conventional and non-conventional, as well as new and emerging sources

With this discussion on simulation techniques and energy security, we decided to handle one real plant design case. The augmentation and efficiency enhancement of an existing 100 MW rated power plant is considered as the objective and study is carried out, which is presented in chapter 2. Various inefficiencies are tackled and enhancement of power is detailed in this chapter 2.

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CHAPTER -2

ENHANCED MODELING AND INTEGRATED SIMULATION OF POWER PLANT FOR CAPACITY ENHANCEMENT AND CLEAN POWER PRODUCTION

The chapter addresses the problem of retrofitting an existing power plant designed to produce 100 MW of power but actually producing only 93 MW power due to limitations in process design and availability of raw material feed. Using Aspen HYSYS®, simulations were carried out for 12 gas samples for different fuel supplies to redesign the fuel gas, flare gas and diesel oil systems. Several process changes were evaluated and pruned to give minimum changes necessary. The findings show that, the available fuel gas can be optimally used by implementing the design considerations and provides higher power generation (131 MW) along with omission of heating skid and incorporation of an additional gas turbine. With significant reduction in energy consumption and enhancement in the efficiency of combustor, the present study makes this process a clean power production technique.

Keywords: power plant design, mathematical optimization, gas turbines, capacity enhancement

2.1 INTRODUCTION

Chemical industries, in general, have undergone significant changes during the past three decades due to the increased cost of energy, increasingly stringent environmental regulations, and global competition in product pricing and quality. One of the most important engineering tools for addressing these issues is optimization. Modifications in plant design and operating procedures have been implemented to reduce costs and meet constraints with an emphasis on improving efficiency and increasing profitability. Optimal operating conditions can be implemented through increased automation at the process, plant, and company levels. As the power of computers has increased, the size and complexity of problems that can be solved by optimization techniques have correspondingly expanded. To apply optimization effectively in the chemical industries, both the theory and practice of optimization must be understood.

Planning and scheduling in chemical industry, particularly in power plants, are resource-intensive and complex processes. Decisions are taken at different stages i.e. supply, production and distribution; and at different levels in the management hierarchy. Every step is vital during the process and hence the flow of information in the operations is quite essential to optimally use the resources as well as produce power as of requirement.

The Combined Cycle Plant (CCP) is a generic type of plant that uses a gas turbine (GT) to produce electric or mechanical power and whose exhaust is used in a heat recovery steam generator (HRSG) that produces steam at different pressure levels [1,2]. The steam can be used in steam turbines for producing additional electricity or mechanical power and/or for the supply of heat loads in a process plant. A sub classification of this system is without steam turbines, well known as a cogeneration plant [3, 4]. Utility systems involving gas and steam turbines have been simulated and optimized using mixed integer linear programming (MILP) [5]; multi-objective optimization of coal-fired power plants [6]; modular simulation [7]; process simulation with an entrained coal gasifier [8]. Efficiency enhancement methodologies have also been discussed earlier [9, 10]. Carbon reduction mechanism with fuel switching was also attempted [11]. However, no application seems to have been reported of the equation modeling, simulation and optimization of CCPs for optimum capacity enhancement involving fundamental models for all the relevant streams, unit operations, investment and operating cost optimization. This forms one of the main objectives of this study. The design of a power plant needs the optimal configuration of process operations and parameters, which can lead to the most economic design. The need of extensive use of such tools in energy engineering applications has been discussed recently [12]. These methods are reviewed as follows:

2.1.1 Thermodynamic approach:

The traditional way of designing power plants is to maximize the thermal efficiency of the plant. For this purpose analysis methods based on both, the first and the second law of thermodynamics, have been extensively discussed in literature [13, 14]. The analysis reveals the thermal inefficiencies of the various subsystems of the plant. Once the inefficiencies have been identified, heuristic rules are applied to improve the performance of the plant. These heuristics form the basis for both parameter and structural modifications to the plant. The capital cost of the plant is assessed after the thermally best design is achieved [15].

This approach gives a good understanding of the process, but it may lead to extensive trial and error in searching for the optimal configuration and set of parameters. It does not take into account the complex interactions between the subsystems. Furthermore, when the economics is discarded at the decision making stage, the most economical performance of the plant may not be achieved [16, 17].

2.1.2 Thermoeconomic approach:

This is an extension of the thermodynamic approach. Capital cost of the units and the prices of product streams of the units are included in the second law analysis model of the plant. This approach tries to address the trade-off between thermal efficiency and capital expenditure. The model is subjected to NLP-optimization for finding the most economic operating parameters. Although this approach provides the economically best parameters, the methodology still relies on trial-and-error, when addressing structural changes to the existing process [18, 19].

2.1.3 Mathematical optimization:

To explore the benefits of both, parameter and structural changes in the process, it may be possible to build a general superstructure containing all the possible process options and subjecting it to optimization [20]. In practice, however, there are several drawbacks associated with this approach. The formulation of power plant processes is inherently non-convex nonlinear by nature, which means that a good initial starting point and feasible bounds for variables must be provided to guarantee a good solution. Secondly, if all the candidate options are included, the number of binary variables may become prohibitive. Therefore, it is essential to find a systematic way of building a superstructure, which includes all the promising alternatives without being too large.

In CC, as coal is not combusted, the relatively small volumes of synthesis gas (syngas) are easier to clean up than the much larger volumes of flue gases at coal combustion plants [21]. Ongoing research activities focus on thermal efficiency enhancement including cost related aspects and environmental performance indicators [22-25]. Higher energy conversion efficiency leads to a better use of coal as the resource and contributes to the reduction of greenhouse gases and other pollutants. Efforts are made to use combined cycle streams for generation of low calorific syngas fuels [26].

Apart from design considerations, Integrated Gas Combined Cycle (IGCC) plant performance depends on numerous integration options and can be improved by process optimization [27-29]. These considerations include:

- Gas turbine air extraction to the air separation unit (ASU).
- Increase the gas turbine power.
- High and low temperature heat recovery.
- Steam generation conditions.
- Utility balance.
- Co-production or polygeneration including steam, hydrogen, and other products.
- Optimization of operating conditions, etc.

This chapter presents an optimization scheme for the existing power plant using three GTGs and a rated fuel gas supply capacity of 27400 Nm^3 /hr for high pressure knockout vessel, gas conditioning skid and filters. The design value of power output for this plant is 100 MW while in practice it produces only 93 MW (see table 2 for other design details). The power company desires to augment the power output and has installed a new fuel development plant unit for supplying pressurized and conditioned fuel gas to the power plant. This unit will provide high fuel gas in excess and thus creates the need to install a new Gas Turbine number 4. The aim of this simulation study is to determine the effect of addition of fourth GTG on the existing system and suggest process changes. The scope of these simulation studies is to design the Fuel gas, Flare gas and Diesel Oil systems and carry out simulations for twelve gas cases as envisaged for different fuel supplies.

2.2 MODEL OF POWER PLANT

Enhanced systems have been proposed for coal based IGCC plants recently [30-32]. As the fuel type for present study differs from the work reported earlier, the power plant model used here has consideration of gas stream composition, gas turbines, heat exchanger skid for Heat Recovery Steam Generator (HRSG), steam drum, and deaerator. The details of each unit considered in the plant are as follows:

2.2.1 Gas stream

Gas stream considered for modeling of gas turbines contain:

- Air (as N_2, O_2 mixture).
- Gas fuel (containing CH_4, C_2H_6, C_3H_8, n-C_4H_{10}, n-C_5H_{12}).
- Exhaust gas components, including products of combustion and dissociation reactions

The stream definition contains N=7 variables (where N is the number of components for a given gas stream). They are F, H, T, P, H, S, y_i (i=1,…,N), respectively representing the molar flow being convenient for modeling the combustion process, enthalpy flow, temperature, pressure, specific enthalpy, specific entropy, and mole fractions.

2.2.2 Gas turbines

Gas turbines represent a complex system consisting of the following three sections:

- a compressor
- a combustion chamber with a pre-mixer for air and fuel; and
- an expansion section.

The model for a gas turbine with above sections is used for simulations earlier [33, 34]. In present study, while modeling the combustion chamber, we first considered the mixing of air from the compressor section with fuel and then a combustion reaction section was modeled. The combustor model requires energy balance and reaction equilibrium equations to calculate the temperature and composition of the combustion products. The combustion products are considered as: N_2, O_2, CO_2, H_2O as well as dissociation products obtained at high temperatures. The expansion section is modeled as a turbine, with a power production term in the energy balance.

2.2.3 Heat exchangers

The exhaust gas of a gas turbine is hot enough to generate steam at different pressure levels for use as process steam. It can also be utilized in deaeration or in steam turbines for additional power generation. A fundamental model was developed for the waste heat recovery section, consisting of a series of heat exchanger models.

2.2.4 Steam drum

A heat recovery steam generator (HRSG) can have several steam pressure levels. A steam drum is required for each pressure level, to separate water from dry steam, which is sent for superheating in the waste heat recovery boiler. The steam drum also helps to stabilize the operation as it connects the streams (water/steam) between the different heat exchange sections into the HRSG and permits an even flow of steam from the HRSG system [35].

2.2.5 Deaerator

This is an important unit operation in utility systems. It eliminates dissolved oxygen in condensate water. In a steam system, raw water makeup is added to compensate for any steam or water losses by purge for steady state operation, including the boiler blow down. Makeup water has a small concentration of dissolved gases (e.g., oxygen and carbon dioxide) and condensate absorbs the dissolved gases after makeup water is induced into the steam system. These dissolved gases produce corrosion in the HRSG heat transfer tubing. Small amounts of oxygen in the steam system can cause severe chemical effects within the system at the operating temperatures.

2.3 SIMULATION OF A FULL GAS TURBINE (GT)

The equipment sections and streams needed to model an open-cycle gas turbine are:

1. The compressor section where air is compressed and then mixed with fuel – in our study, natural gas; 2. the combustion chamber where fuel is burnt with a high excess of oxygen at high temperature (around 1200 °C) and high pressure (above 2.8 MPa); and 3. The expansion section, where the combustion gases are expanded to produce shaftwork for electric power generation as well as mechanical power to drive the compressor section of the gas turbine.

2.3.1 Operating parameters of fuel system for GTG:

The operating and design parameters used for gas turbine operations are shown in table 2.1.

Table 2.1: Gas Turbine operating parameters

Design Capacity (m^3/hr)	**Pressure (barg)**		**Temperature (^oC)**	
	Operating	**Design**	**Operating**	**Design**
11.37	7.5	13.5	50	95

Following the procedure described as well as referred [34], we first simulated this equipment in its individual sections due to the complexity of the combustion chamber model. This was the most difficult subsection to converge since the equations relating the combustion temperature and compositions including dissociation reactions are highly non-linear [36]. The chemical reactions involved in the process are very complex due to involvement of many components. Also, there is a network of irreversible consecutive and competitive reactions. The model uses an approach to represent the reaction as a lumped one and trace reaction products like CS_2 etc., are not considered. The reactors are modeled with the Aspen HYSYS® built in model of Gibbs and Equilibrium Reactors.

2.3.2 Combustion reactions

This model assumes the use of natural gas with the first five alkanes (methane, ethane, propane, *n*-butane and *n*-pentane), identified as $C_l,\dots,C_5$, respectively. The combustion in air of each of these five hydrocarbons is described by an extent of reaction ε_i, $i=1,\dots,5$.

$$\left[C_iH_{2i+2} + \frac{3i+1}{2}O_2 \longrightarrow iCO_2 + (i+1)H_2O\right]$$

These extents were determined by the fuel gas conversion being set to equal the combustion efficiency for each natural gas component.

2.3.3 Equilibrium reactions

When the products of a combustion reaction are at temperatures above 1100 °C, there is significant chemical dissociation of the constituent gases. For possible high temperature combustion, the present model includes dissociation reactions [37] which are assumed to be at equilibrium in order to give the correct specific enthalpy and composition of the product stream. These reactions have extents of reaction designated as ε_i, $i=1, \dots, 6$, respectively for the 6 reactions:

$$CO_2 \leftrightarrow CO + \frac{1}{2}O_2 \text{..................}(1)$$

$$\frac{1}{2}O_2 + \frac{1}{2}N_2 \leftrightarrow NO \text{.................}(2)$$

$$H_2O \leftrightarrow H_2 + \frac{1}{2}O_2 \text{..................}(3)$$

$$H_2O \leftrightarrow \frac{1}{2}O_2 + OH \text{.................}(4)$$

$$H_2 \leftrightarrow 2H \text{.................................}(5)$$

$$O_2 \leftrightarrow 2O \text{.................................}(6)$$

However, if the turbine inlet temperature is assumed to be less than 1500 °C, then only the first two equilibrium reactions for CO and NO formation can be considered [38, 39]. In reality other oxides of nitrogen may also form, but this model lumps them together.

2.4 METHODOLOGY

The Gas Turbine combustion system is of dual fuel type which is designed to burn both the fuels, Natural Gas and Diesel Oil, with automatic control. Fuel changeover shall be initiated manually through the fuel selector switch or automatically by the fuel gas pressure switch which is operated when the fuel gas pressure drops below a preset value. Fuel gas (Natural gas) is presently the primary source of fuel for the power plant. This comes from offshore and onshore fuel gas production facilities.

As a part of detailed engineering for this extension Gas Turbine Generator unit in this power plant, a simulation study and calculations are carried out for the following systems:

(i) Fuel Gas System
(ii) Flare System
(iii) Diesel Oil System

The complete process flow diagram developed for the simulation study is shown in figure 2.1. In the first instance, we have generated the complete process for three gas turbines. The bottlenecks in producing optimal power were identified. This information from the design and simulation study was used to suggest process changes including installation of fourth gas turbine. The additional changes in the process flow diagram are indicated through dashed outlines and include removal of fuel heaters for non hydrate formation conditions and addition of fourth gas turbine generator for capacity augmentation.

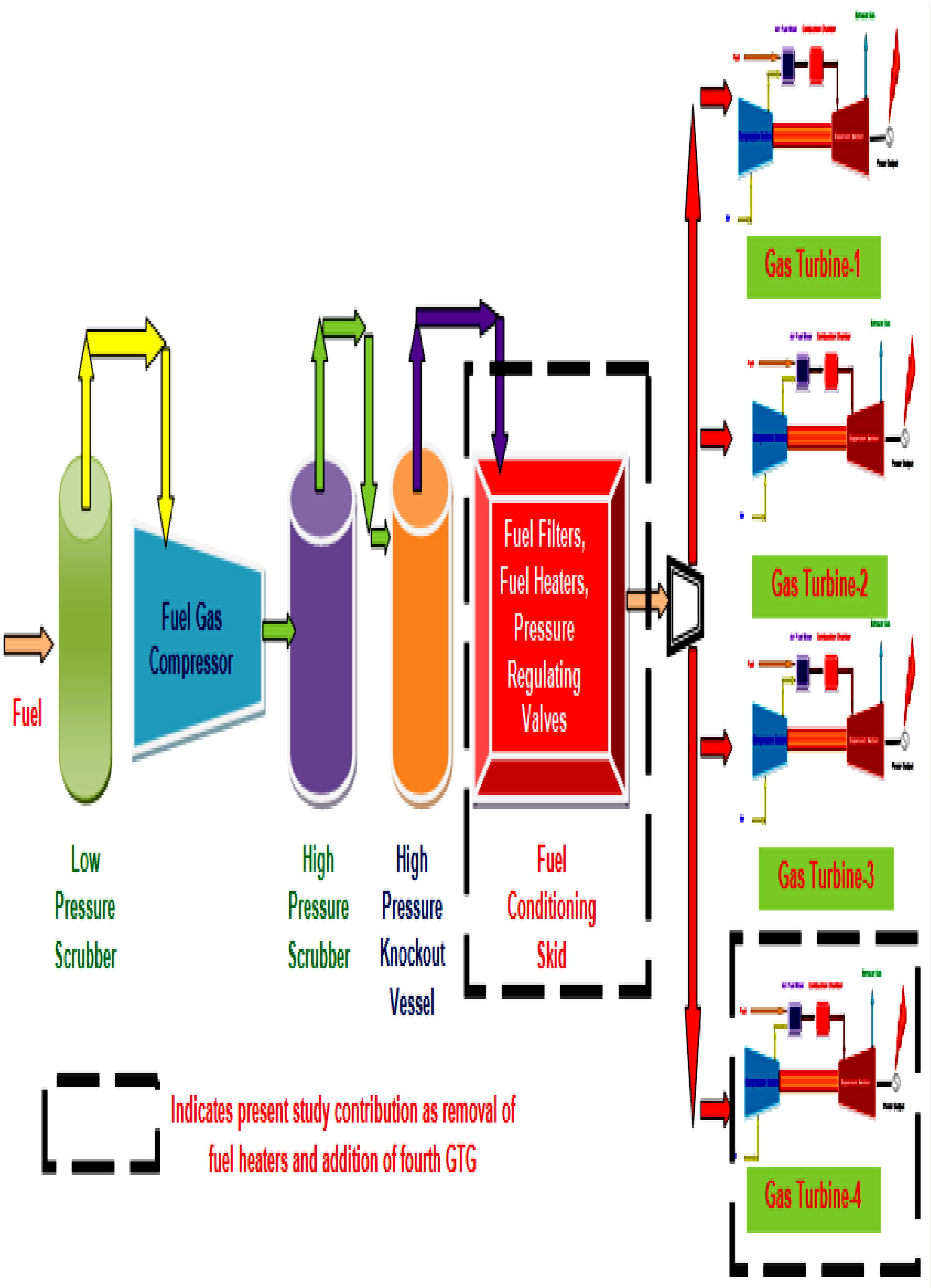

Fig. 2.1: Process Flow Diagram developed for simulation of the power plant

The complete power generation process system as envisaged in the present study and later simulated is described below:

2.4.1 Fuel Gas System:

The fuel gas (Natural gas) is presently the primary source of fuel for the power plant. Currently, the fuel gas system comprises of a low pressure scrubber, fuel gas compressors, high pressure scrubber, high pressure knockout vessel and a gas conditioning skid (composed of fuel filters, fuel heaters and pressure regulating valves). The gas conditioning package is a compact self contained skid which provides removal of liquid particles from the fuel gas, temperature control and pressure regulation (22 barg) of the fuel gas before it is fed to the gas turbines. A new gas processing plant supplies compressed and treated gas ready to be used for power plant as fuel. The gas is fed to the Gas Turbines through the fuel gas conditioning skid. Estimated flow availability of the conditioned gas for three GTGs operating at 50 ^{o}C and generating a total of 100 MW as rated capacity is 49517 Nm^3/hr.

2.4.2 High Pressure Knockout Vessel:

There is one High Pressure Knockout Vessel of vertical demister type, which has a design flow rate of 47400 Nm^3/hr and design pressure and temperature are 34 barg and 160 ºC respectively. The High Pressure Knockout Vessel is designed for a liquid slug that can occur due to an upset condition in upstream operation of the gas system.

2.4.3 Fuel Gas Conditioning Skid:

Fuel Gas Conditioning Skid is located near the Gas Turbine area. It consists of Fuel Gas Filter Separator, Fuel Gas Super heaters and Pressure Regulating Valves. The gas conditioning package provides removal of liquid particles from the fuel gas, temperature control and pressure regulation of the fuel gas before it enters the gas turbine. Design flow for the present fuel gas system is 47400 Nm^3/hr that consists of three Gas Turbines operating at base load and 50 ºC $^{+}/_{-}$ 10% contingency.

2.4.4 Fuel Gas Filter Separator:

There are two horizontal type Fuel Gas Filter Separators having filter size not greater than 3µm. Each Fuel Gas Filter Separator is designed for a gas flow of 47400 Nm^3/hr. Design pressure and design temperature are 34 barg and 160 ºC respectively.

2.4.5 Fuel Gas Super Heater:

There are three electric immersion type Fuel Gas Super Heaters, each having thermal output of 303 kW. Each super heater has design flow rate of 16600 Nm^3/hr and design pressure and temperature are 34 barg and 160 ºC respectively.

2.4.6 Pressure Control Valve:

There are four control valves. Two valves in series are deployed on two parallel paths. Normally one set of valves on one path remains in service and the other set of valves on the second path remains as standby. For the set of control valves in operation, normally the upstream valve remains FULLY OPEN and the downstream valve modulates to maintain a downstream pressure of 22.5 barg. If the downstream control valve fails to maintain the downstream pressure, the upstream control valve takes over the operation and regulates to maintain a downstream pressure of 22 barg. During this change over, the downstream pressure control valve remains OPEN. Design capacity of each control valve is 29000 Nm^3/hr. The maximum quantity of fuel gas supply handling capacity is around 55630 Nm^3/hr at 28.66 barg.

In the present study, two more control valves are suggested to be used in series on a parallel path to the above mentioned set of control valves. These are not available in the existing plant. They are of smaller size and are utilized for initial charging of the Fuel Gas System and start–up of the Gas Turbines. These valves are set to regulate the downstream pressure at 23.5 barg.

The existing gas turbine combustion system is dual fuel type which is designed to burn both, the natural gas and diesel oil. In the present work, we introduced an additional fourth Gas Turbine Generator of GE Frame 6 model which is also designed for dual fuel continuous operation with automatic control. Diesel oil is normally used during start-up and as back-up fuel. Fuel gas is considered as the primary fuel. We designed the fuel system such that fuel changeover will be initiated manually through the fuel selector switch or automatically by the fuel gas pressure switch which starts operating when the fuel gas pressure drops below a preset value.

The design capacities of the above components of fuel gas system can process gas fuel of 47400 Nm^3/hr, whereas the available maximum fuel supply is only 35630 Nm^3/hr. Thus, although higher design capacity equipment are available in the existing plant, all these units cannot be utilized to their full design capacity due to fuel gas supply limitations. A detailed comparison of existing plant parameters to the modified parameters for various unit components of fuel gas conditioning system is provided in table 2.2. This explains the implementation of the methodology adopted in the present work for the capacity enhancement.

Table 2.2: Existing design capacities and design modifications in the system

Components of Fuel Gas System	**Present Design Capacity, Nm^3/hr**	**Actual usage in practice, Nm^3/hr**	**Modified Design usage capacity, Nm^3/hr**	**Power generation, MW**	
				Existing Plant	**Modified Plant**
Fuel Gas System	49517	27400	35630	93	131
High Pressure Knockout Vessel	47400	27400	35630		
Fuel Gas Conditioning Skid	47400	27400	35630		
Fuel Gas Filter Separator	47400	27400	35630		

Fuel Gas Super Heaters (Each of Three Units)	16600	9130	11900		
Pressure Control Valves	29000	27400	58000 (Two sets)		

The modifications suggested in table 2.2 do not require drastic changes in the existing infrastructure of the plant. With the simulation results shown in table 2.3, it is endorsed that higher power production is feasible.

Table 2.3: Effect of design modifications on power generation

Units in Fuel Gas System	**Present Design Capacity, kg/hr**	**Actual usage in practice, kg/hr**	**Modified design capacity, Nm^3/hr**	**Power generation, MW**	
				Existing Plant	Modified Plant
GTG-1	9000	8550	8494	**35.5**	35.42
GTG-2	9000	8550	8494	**35.5**	35.42
GTG-3	9000	8250	8494	**34.0**	35.42
GTG-4	Not present	Not present	5518	**Not present**	23.22

Various unit operations used in simulation of full power plant with their design models in simulators are shown in table 2.4. The appropriate choices of simulation models have helped in optimization of efficiency of gas turbines as well as compressors. The parameters derived from design studies which are used for performing the simulations are provided in table 2.5. The gas turbine is modeled as per the parameters and the sections demonstrated in figure 2.2 (see also [40]).

Table 2.4: Representative unit operations used in the simulation of the power plant

Unit Operation	Aspen HYSYS® Model
Combustor	Gibbs Reactor
Air Compressor	Compressor
HRSG	LNG Exchanger
Gas Turbine	Expander

Table 2.5: Parameters for simulation of the power plant

Process	Parameters	Values
Gas Turbine	**Power (Design)**	**100 MW**
	Inlet Temperature	**1421 °C**
	Isentropic Efficiency	**93.3 %**
GT Compressor	**Pressure Ratio**	**9.09**
	Isentropic Efficiency	**59.99 %**

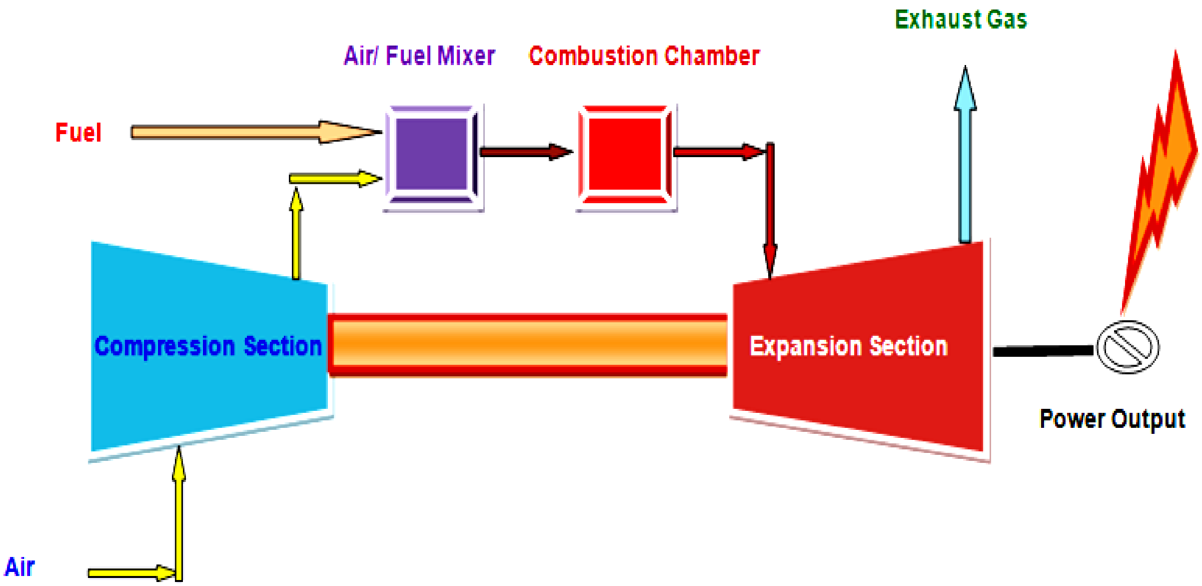

Fig. 2.2: Sections and streams in gas turbine modeling study

2.5 SIMULATION MODEL: RESULTS AND OUTCOMES

The results of process simulation study and calculations performed are provided below. The equation-oriented approach adopted in the present study has helped in controlling the reactions in the combustion chamber, leading to thermal efficiency enhancement. This is achieved by keeping the temperature below 1500 ^{0}C. Tables 2.6 and 2.7 indicate the parameters and best conditions achieved by simulation for two different gas samples. Complete study has been carried out with all such twelve gas samples in twelve different simulation cases as an effort towards clean power production system. Efficiency enhancements are reported by alternate methods in current years [41, 42] which require drastic changes. This emphasizes the contribution of present study in optimizing the power generation capacity efficiently in an existing plant without changing production routes. This has not been done before.

Table 2.6: Total power generation in each GTG with additional 4th GTG for Normal Mode Case: 17 % Water Cut (WC), 50 ^{0}C and 100% RH

Turbine Parameters	Units	GTG1	GTG2	GTG3	GTG4
Fuel Gas mass flowrate	kg/hr	8494	8494	8494	5518
Vapour Fraction	-	1	1	1	1
Liquid Fraction	-	0	0	0	0
Temperature	^{0}C	51.64	51.64	51.64	51.64
Pressure	kPa	2301	2301	2301	2301
LHV	kJ/kg	47310	47310	47310	47310
HC Dew Point (Gas)	^{0}C	-39.63	-39.63	-39.63	-39.63
Water Dew Point (Gas)	^{0}C	-260.5	-260.5	-260.5	-260.5
Compressor Power (consumed) x 10^7	kJ/hr	28.33	28.33	28.33	18.40

Heater Power (consumed) x 10^5	kJ/hr	10.908	10.908	10.908	0
Turbine Power (Generate) x 10^7	kJ/hr	41.19	41.19	41.19	26.76
Total Power Generation x 10^7	kJ/hr	12.75	12.75	12.75	8.36
Total Power Generation X 10^3	kW	35.42	35.42	35.42	23.29
Total Power Generation	**MW**	**129.49**			

Table 2.7: Total power generation in each GTG with additional 4th GTG for Normal Mode Case: 50 % Water Cut (WC), 50 ^{0}C and 100% RH

Turbine Parameters	**Units**	**GTG1**	**GTG2**	**GTG3**	**GTG4**
Fuel Gas mass flowrate	kg/hr	8494	8494	8494	5518
Vapour Fraction	-	1	1	1	1
Liquid Fraction	-	0	0	0	0
Temperature	^{0}C	52.23	52.23	52.23	52.23
Pressure	KPa	2301	2301	2301	2301
LHV	KJ/kg	47340	47340	47340	47340
HC Dew Point (Gas)	^{0}C	-39.63	-39.63	-39.63	-39.63
Water Dew Point (Gas)	^{0}C	-260.5	-260.5	-260.5	-260.5
Compressor Power (consumed) x 10^7	kJ/hr	28.33	28.33	28.33	18.39
Heater Power (consumed) x 10^5	kJ/hr	10.90	10.90	10.90	0.0

Turbine Power (Generate) x 10^7	kJ/hr	41.21	41.21	41.21	26.77
Total Power Generation x 10^7	kJ/hr	12.77	12.77	12.77	8.380
Total Power Generation X 10^3	kW	35.47	35.47	35.47	23.29
Total Power Generation	**MW**	**129.69**			

The complete power plant designed as above including full fuel gas system and four gas turbines is simulated and optimized for power and efficiency enhancement using the simulator. Figures 2.3, 2.4 and 2.5 illustrate the simulation flow diagrams of fuel gas system with their subsections.

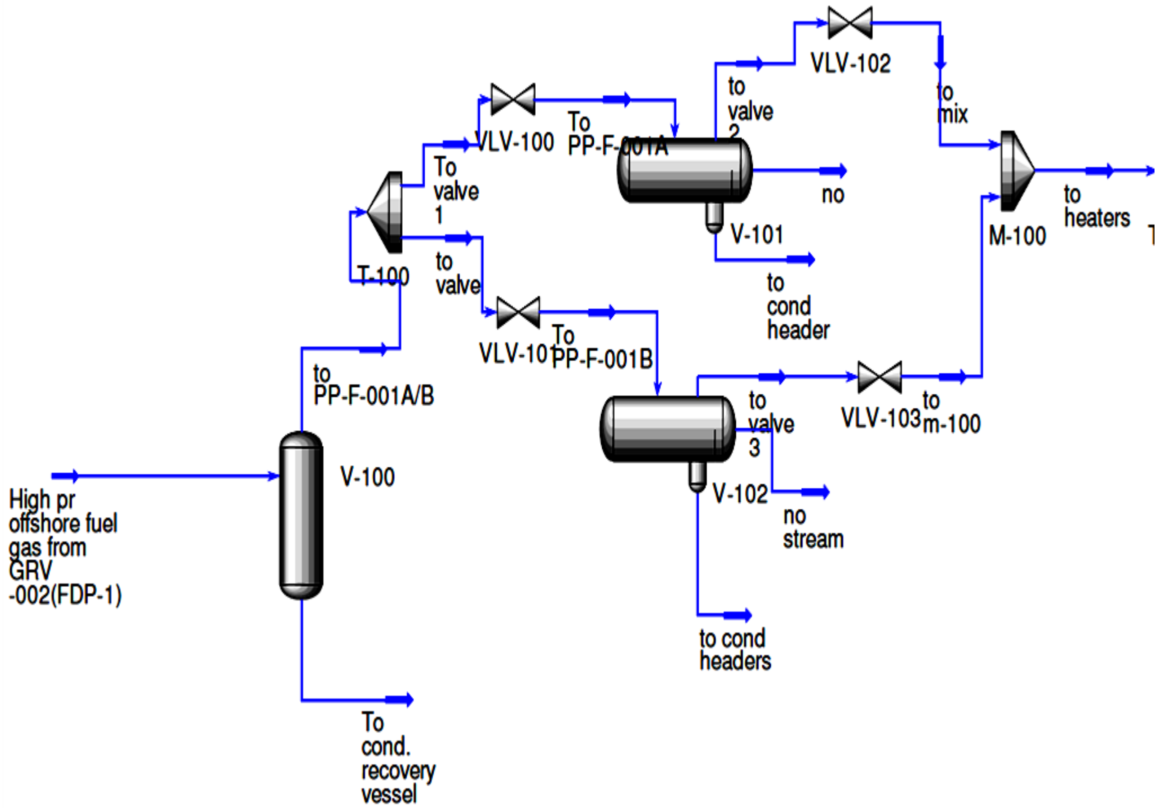

Fig. 2.3: Simulation of fuel gas and high pressure knockout vessel along with scrubbers

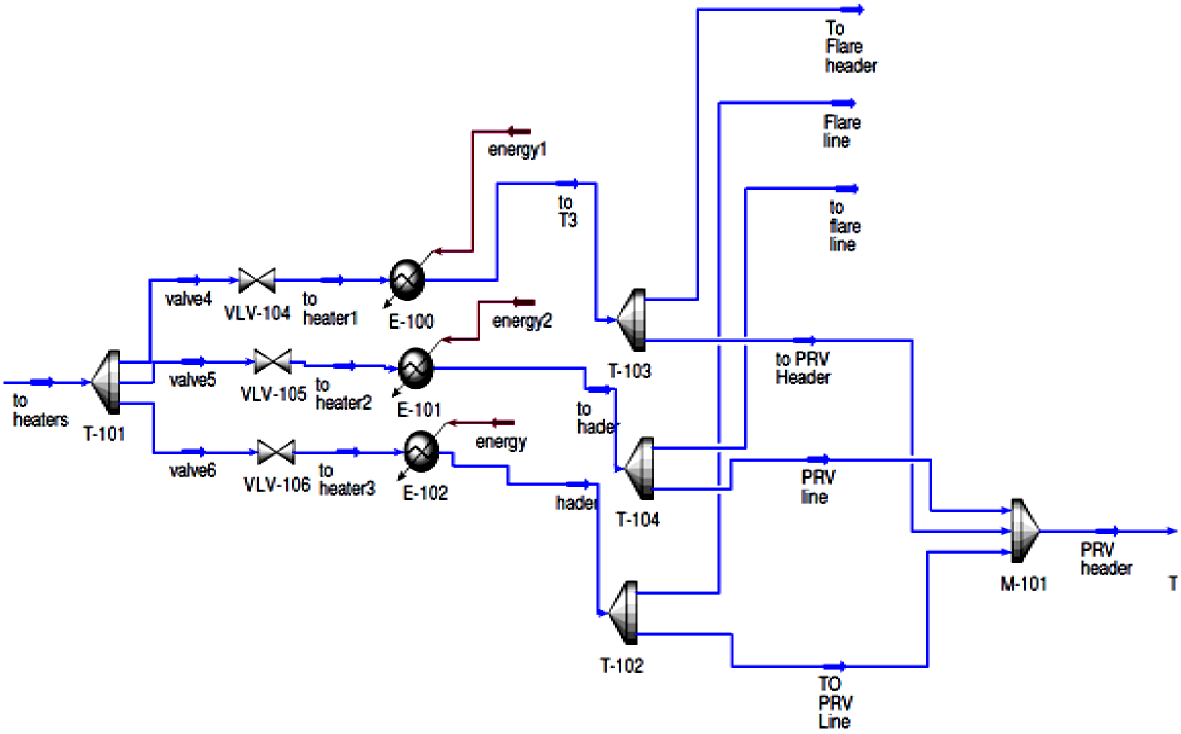

Fig. 2.4: Simulation of heat conditioning skid

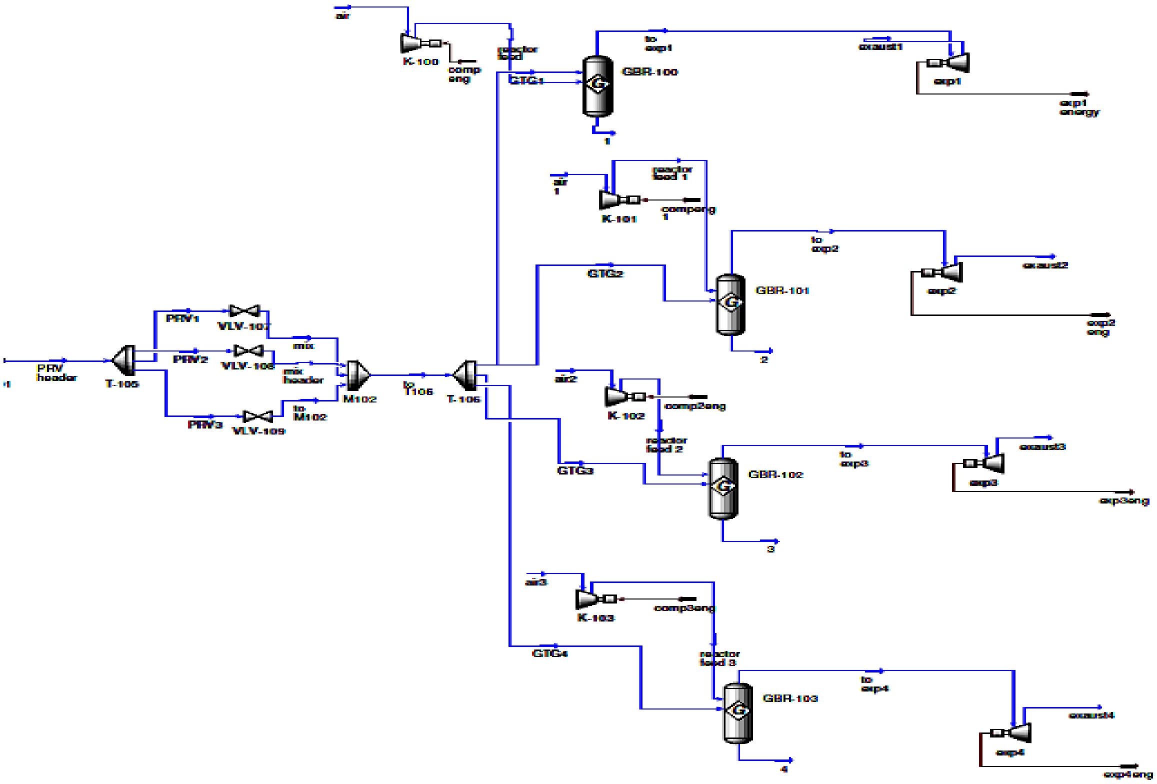

Fig. 2.5: Simulation of gas turbine section with PRVs for capacity augmentation

2.5.1 Analysis and comparison of models of existing and new power generation systems:

2.5.1.1 Analysis with three GTGs:

Maximum power (design) that can be generated: 105 MW (35 MW each)

Required fuel supply: 35630 Nm^3/hr (31000 kg/hr)

The bottlenecks identified in the model developed for existing power plant are:

1. The present high pressure knockout vessel, gas conditioning skid, and filters can process a maximum of 27400 Nm^3/hr (25350 kg/hr) fuel gas only

2. Fuel gas super heating with two heaters is not sufficient. Third heater should be placed in operation. Considering the heating load, the third heater will operate partially and this will hamper the efficiency by around 12%. In present situation, there is no stand by heater in the system. This condition calls for installation of fourth heater which is to be provided as a stand by heater. This is capital intensive.

At present fuel flow rate, due to various inefficiencies the power plant is generating 93 MW (31 MW each) as against the modified design value of 105 MW. In the event we are able to overcome the bottlenecks mentioned under (1) and (2), a possible simulated scenario is presented in table 2.8. The numbers in parenthesis are practically possible values at present whereas the numbers without brackets indicate simulated results. In order to realize these numbers in practice, drastic changes in feeding systems and other utility lines will be required besides shut down and down-time and is not a feasible solution. An alternative with four GTGs is thus suggested, which suites the need of the plant.

Table 2.8: Total power generation in each GTG with 3 GTGs i.e. without additional 4th GTG

Gas Analysis		Parameters	Units	GTG1	GTG2	GTG3	GTG4
1	17% WC	Gas flow	Kg/hr	11350 (8550)	11350 (8550)	8308 (8250)	0
		LHV	kJ/kg	47340	47340	47340	0
		Power generated	MW	47.94 (35.5)	47.94 (35.5)	35.41 (34.0)	0
		Total Power, MW	**131.29 (105)**				
2	35% WC	Gas flow	Kg/hr	11350 (8550)	11350 (8550)	8308 (8250)	0
		LHV	kJ/kg	47360	47360	47360	0
		Power generated	MW	47.94 (35.5)	47.94 (35.5)	35.47 (34.0)	0
		Total Power, MW	**131.35 (105)**				
3	50% WC	Gas flow	Kg/hr	11350 (8550)	11350 (8550)	8308 (8250)	0
		LHV	kJ/kg	47380	47380	47380	0
		Power generated	MW	48.04 (35.5)	48.04 (35.5)	35.51 (34.0)	0
		Total Power, MW	**131.59 (105)**				

2.5.1.2 Analysis with four GTGs:

Maximum power (design) that can be generated: 131 MW, with full load and partial one

Available fuel supply: 35630 Nm^3/hr (31000 kg/hr)

Bottlenecks and their solutions implemented for the new design are explained below:

1. The present high pressure knockout vessel, gas conditioning skid, and filters are able to process a maximum of 27400 Nm^3/hr. This has been overcome by using two parallel sets of operations as mentioned earlier in Section 2.4.

2. Direct flow is essential for the required power generation. The simulation can accommodate the direct flow.

3. With four GTGs, a maximum of 105 MW power can be generated with existing line conditions. PRVs are not able to run fourth GTG at full speed. This bottleneck is also removed in the present study by using the second set of PRVs. Hence, power generation capacity can now be augmented to 131 MW.

At present flow rate, with the required changes incorporated, the power plant is now producing a maximum power of 131 MW.

The effects of twelve gas samples on power production at defined conditions have been assessed. The simulation conditions for normal mode for three gas analyses, as indicative results, are reported in table 9. With these modifications, enhancement in power generation is obvious.

Table 2.9: Final power generation in each GTG with additional 4th GTG

Gas Analysis		**Parameters**	**Units**	**GTG1**	**GTG2**	**GTG3**	**GTG4**
1	17% WC	Gas flow	Kg/hr	8494	8494	8494	5518
		LHV	kJ/kg	47310	47310	47310	47310
		Power generated	MW	35.68	35.68	35.68	23.22
		Total Power, MW	**130.26**				
2	35% WC	Gas flow	Kg/hr	8494	8494	8494	5518
		LHV	kJ/kg	47320	47320	47320	47320
		Power generated	MW	35.78	35.78	35.78	23.24
		Total Power, MW	**130.58**				
3	50% WC	Gas flow	Kg/hr	8494	8494	8494	5518
		LHV	kJ/kg	47340	47340	47340	47340
		Power generated	MW	35.78	35.78	35.78	23.27
		Total Power, MW	**130.61**				

Figure 2.6 illustrates the simulated process flow diagram with four GTGs, which is a simulation case for augmented capacity.

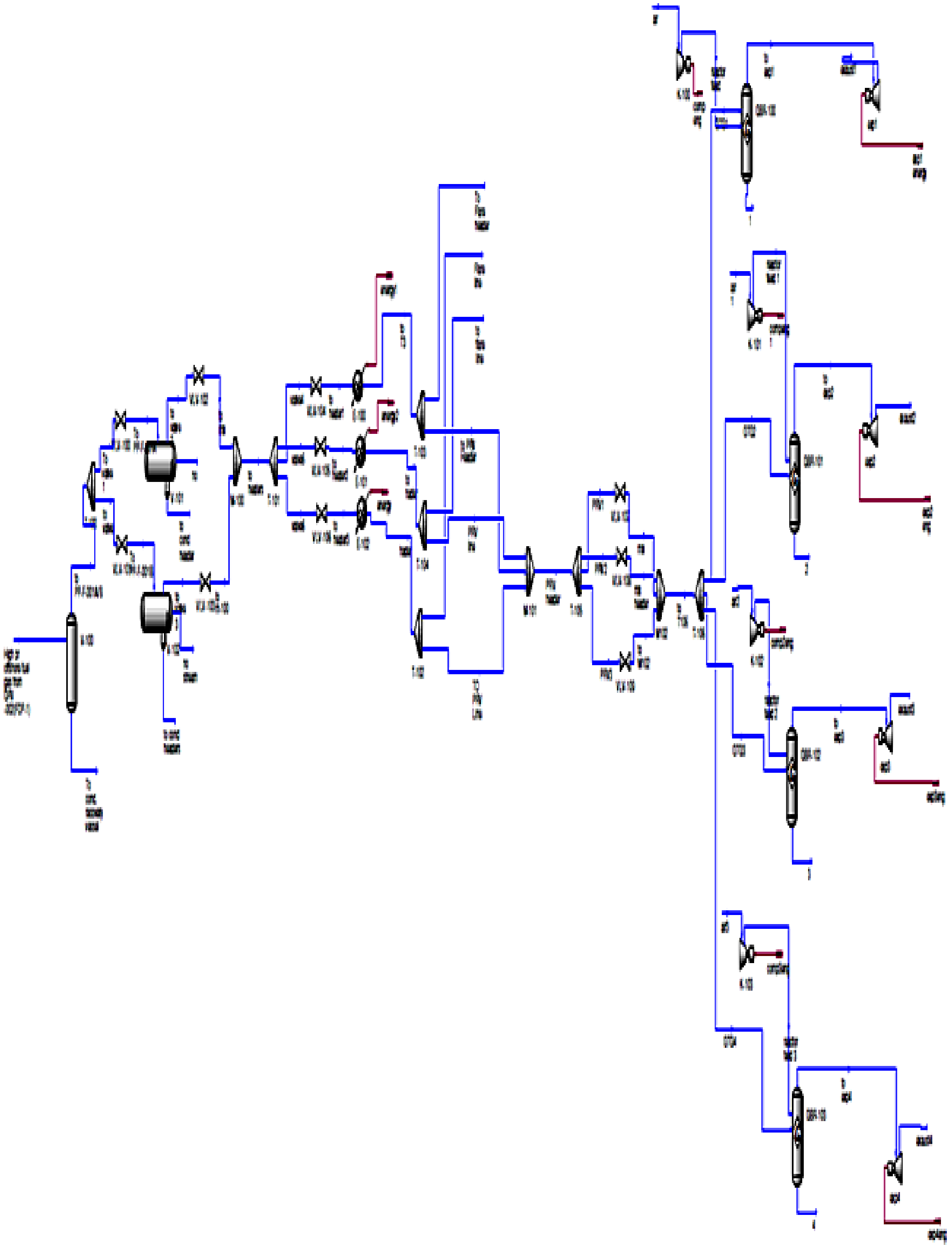

Fig. 2.6: Complete simulation of fuel gas system with four GTGs

2.5.2 Other modifications:

The flow and pressure drop analysis of the system by direct suction header indicates that, under present condition, bypass of tanks is controlled solely by the orifice. An effective model was developed where the system is controlled by a combination of an orifice and a control valve.

In Diesel Oil system, pressure drop calculations are carried out for flow from tank back to pump with a recycle flow of 50 m^3/hr. The pressure drop across the orifice under conditions of 1GTG to 4GTGs varies from 48.432 m to 51.122 m. This is quite within a narrow range. Therefore, this scheme is practical to operate. This rearrangement in present study makes the duel fuel operating system more reliable and steadily operating.

Gas hydrate formation is shown as a possible scenario by the simulation. Same is the case for Full Speed No Load (FSNL) condition at GTG4 inlet. The gas conditioning skid deployed in the present study removes this possibility and thus enhance the gas turbine operability. Present study recommends only essential use of heating skid to avoid hydrate formation, otherwise skips the heating skid and saves more energy.

Comparison of models for existing power generation system with three gas turbines to newly designed power generation system with four gas turbines is represented in figures 2.7 and 2.8. These figures indicate total power enhancement and hence prove the successful augmentation of capacity of present plant without any addition of fuel requirement. This also underlines the success and effectiveness of this simulation study.

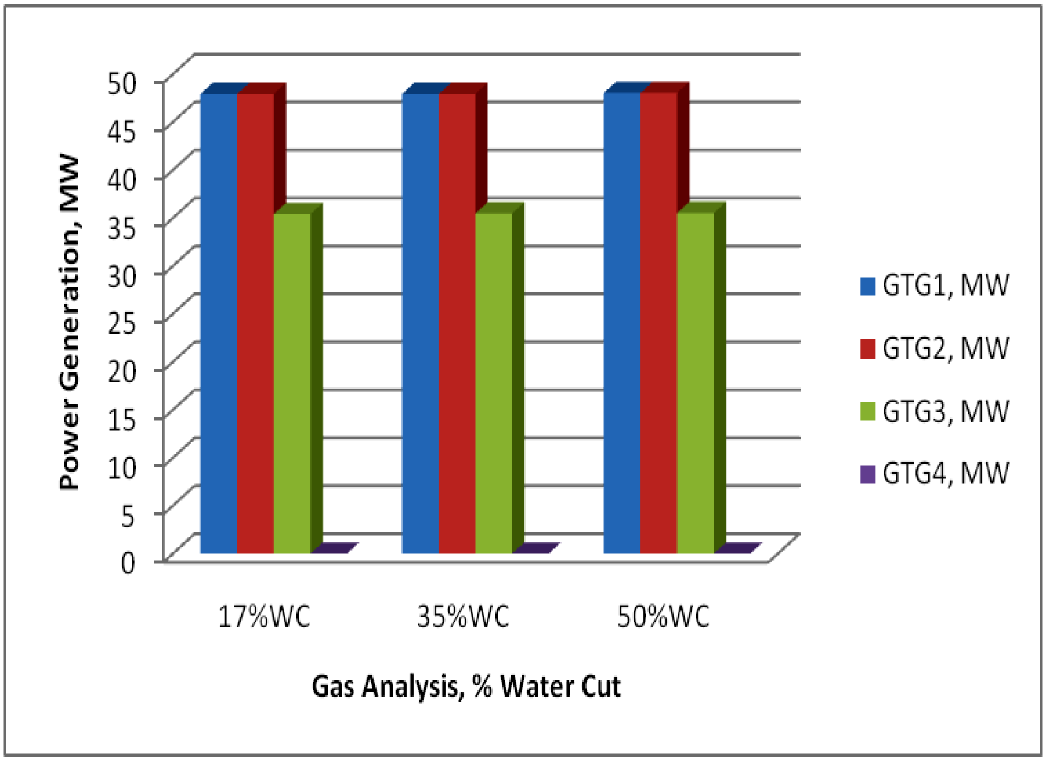

Fig. 2.7: Total power generation with three GTGs for three gas analyses

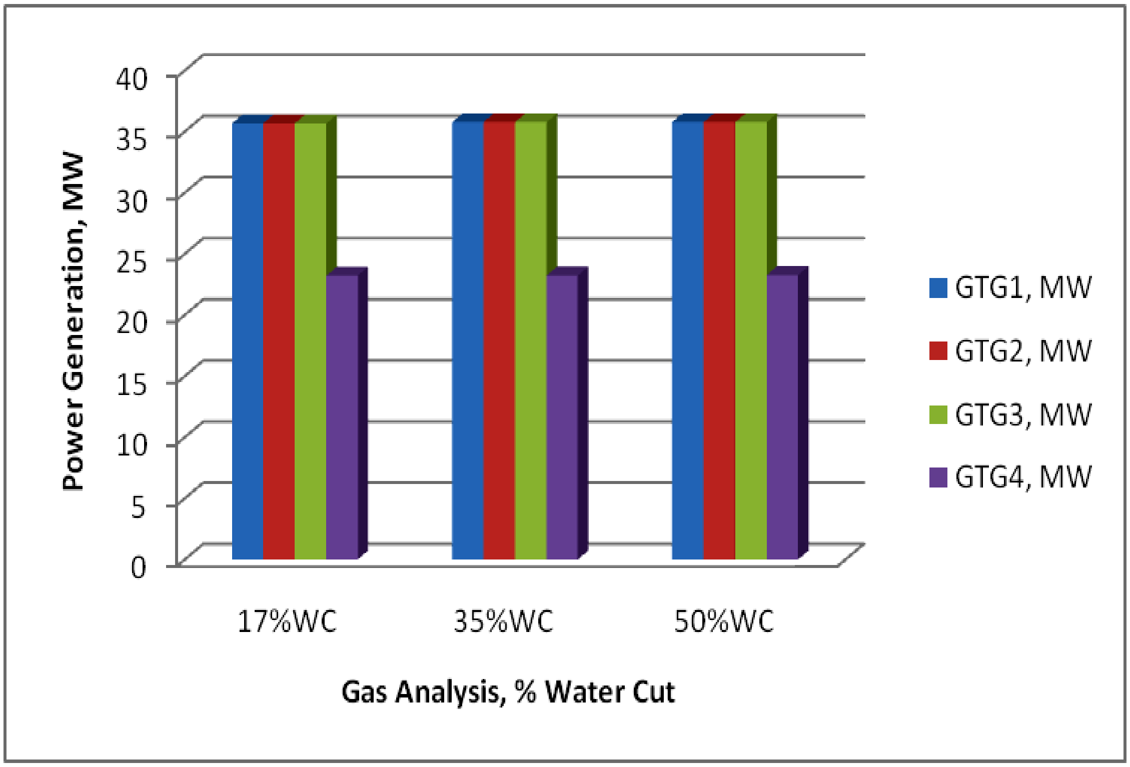

Fig. 2.8: Total power generation with four GTGs for three gas analyses

Some of the additional results for winter and summer conditions are demonstrated by figures 2.9 and 2.10. The figures show that, in any condition and with any gas sample, the individual power production in each GTG is not hampered. This is an important observation which enhances the operational feasibility of the plant and endorses the robustness of the model developed and simulated in the present study.

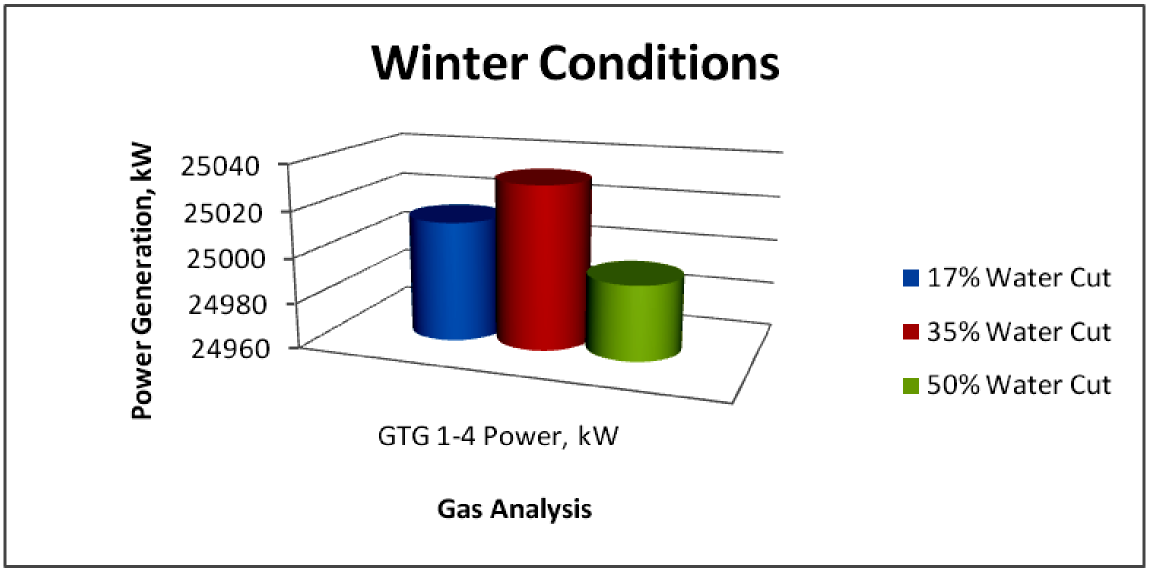

Fig. 2.9: Effect of humidity on power generation: winter conditions

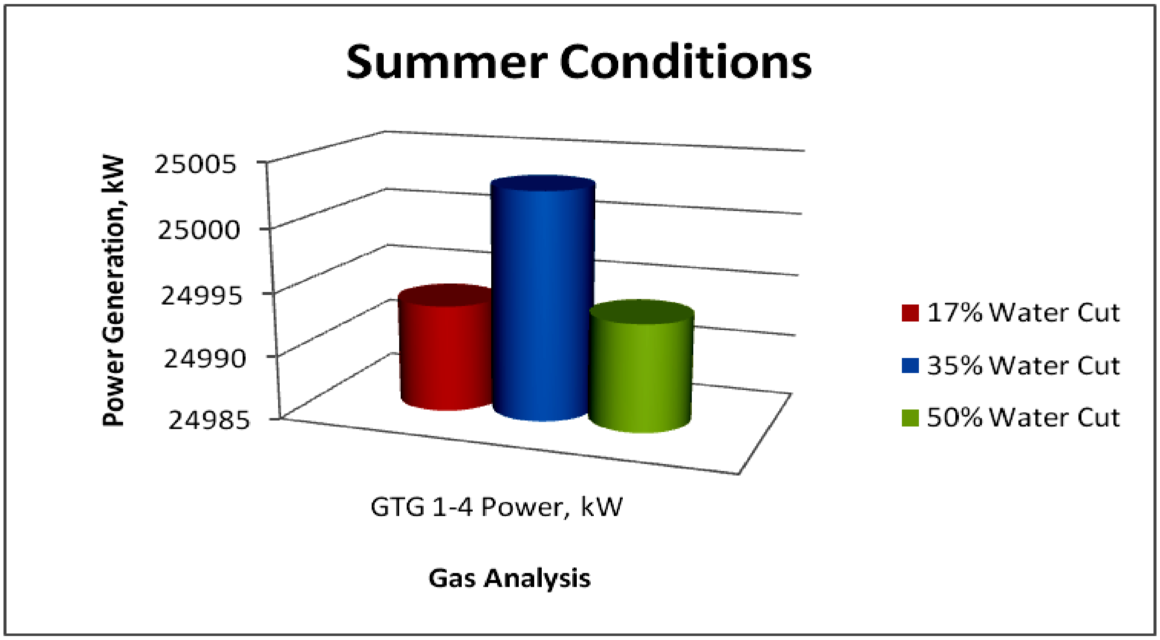

Fig. 2.10: Effect of humidity on power generation: summer conditions

CONCLUSIONS

The newly installed fuel gas system has the capacity to deliver 55360 Nm^3/hr of fuel gas flow. The design capacities of various units of fuel gas system are, however, limited to 47400 Nm^3/hr. Full utilization and maximum power generation will require drastic design changes. Presently, the fuel supply is constrained to 35630 Nm^3/hr due to limited availability of feed stock raw material. All calculations are therefore carried out for this limiting case. Fuel supply modifications, such as by-passing the heater skid, save energy on heating the gas to the tune of electric power of 900 kWh. Maximum possible power generation in four GTGs is approximately 131 MW. The existing power plant could produce only 93 MW with 31 MW each for three GTGs. This enhancement in efficiency and augmentation is achieved by increasing the fuel gas flow from 27400 NM^3/hr to 35630 NM^3/hr. Pressure control valves have been modified to accommodate the full gas flow required due to addition of one more GTG. The gasifier efficiency is enhanced using lumping parameter models for reactions by maintaining inlet temperature below 1500 ^oC. This helps the complete conversion of CO and NOx, which in turn reduces pollution and makes this as a process of clean power production.

Simulation results including gas property estimations have been worked out. Dew Point Control Unit (DPCU) mode gas has a higher content of C_3 and C_4 fraction against normal mode. Therefore gas requirement is lower in this mode of operation. Under winter condition in DPCU mode, gas hydrate formation possibility is indicated. This shows that the thermodynamic conditions favour hydrate formation. So, if the gas is conditioned and maintained dry as illustrated in the present study, the hydrate formation possibility can be removed totally making this as a route for safer and cleaner enhanced power production.

As the real plant case study was successfully carried out, we decided to look back to the fluidized bed gasification technology, which is experiencing many resistances due to various inefficiencies. The detailed literature survey is performed along with optimization of design and simulation calculations for various capacities of fluidized bed coal gasification process. The details are discussed in chapter 3.

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CHAPTER -3

MODELING, DESIGN AND SIMULATION OF FLUIDIZED BED COAL GASIFIER

Fluidized bed gasification is one of the potential sources for production of clean and eco-friendly fuel. With the gradual depletion of coal and petroleum resources biomass is being perceived as a self-sustainable source of energy production. Concerns about climate change and economic forces have made the need for clean energy from fossil and biomass fuels more important than ever. This has brought an attention on gasification to supplement fossil fuelled energy, particularly by a fluidized bed. Developing tools and methods to predict operation and performance of gasifier will lead to more efficient gasifier designs. This basic study investigates bed fluidization and particle decomposition for fluidized materials. Effects of particle density and diameter on the minimum fluidization velocity were investigated; a method was developed to predict hydrodynamic response of binary beds from the response of each particle type and mass. This topic contains calculations and results of various parameters such as minimum fluidization velocity, fluidization velocity (U_f), cross sectional area, volumetric flowrates, minimum fluidization height, TDH, total height of the column, and bubble dynamics. Simulation using Aspen *HYSYS*$^{®}$ *is also performed to enhance the H_2/CO ratio from 1.5 to 3.3 and results are produced.*

Keywords: Coal Gasification, Combustion, Fluidized Bed Gasifier, Enhancement in H_2/CO ratio

3.1 INTRODUCTION

Gasification technologies have been commercially applied for more than a century for the production of both, fuels and chemicals. Current trends in the power generation and refinery Industries support the observation that advanced stages of the technology will continue to be applied towards the synthesis of syngas, with an increasing number of applications in power generation, fuels, and basic chemicals manufacturing. Attractive features of technology include [1]:

- The ability to produce a consistent product that can be used for the generation of electricity or as primary building blocks for manufacturers of chemicals and transportation fuels.
- The ability to process a wide range of feed stocks including coal, heavy oils, petroleum coke, heavy refinery residuals, refinery wastes, hydrocarbon contaminated soils, biomass, and agricultural wastes.

3.1.1 GASIFICATION PRINCIPLES: AN OVERVIEW [2, 3]

Gasification is a process for converting carbonaceous materials to a combustible or synthetic gas (e.g., H_2, CO, CO_2, and CH_4). In general, gasification involves the reaction of carbon with air, oxygen, steam, carbon dioxide, or a mixture of these gases at 750 °C or higher to produce a gaseous product that can be used to provide electric power and heat or as a raw material for the synthesis of chemicals, liquid fuels, or other gaseous fuels such as hydrogen.

Figure 3.1 shows the principal methods for gasifying a carbonaceous material.

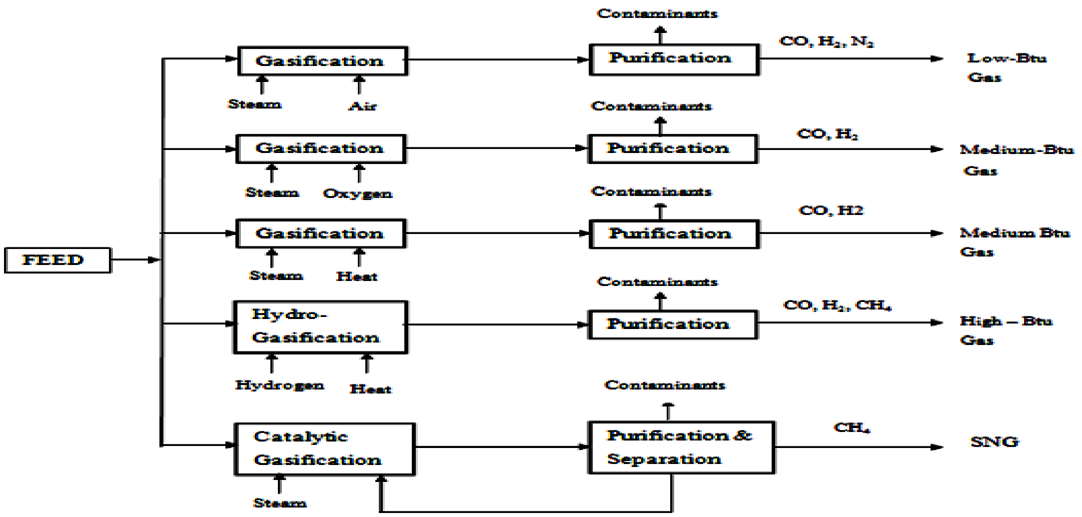

Fig. 3.1: Various gasification methods [2]

Applications of gasification fuels in power and chemical manufacturing is illustrated in figure 3.2.

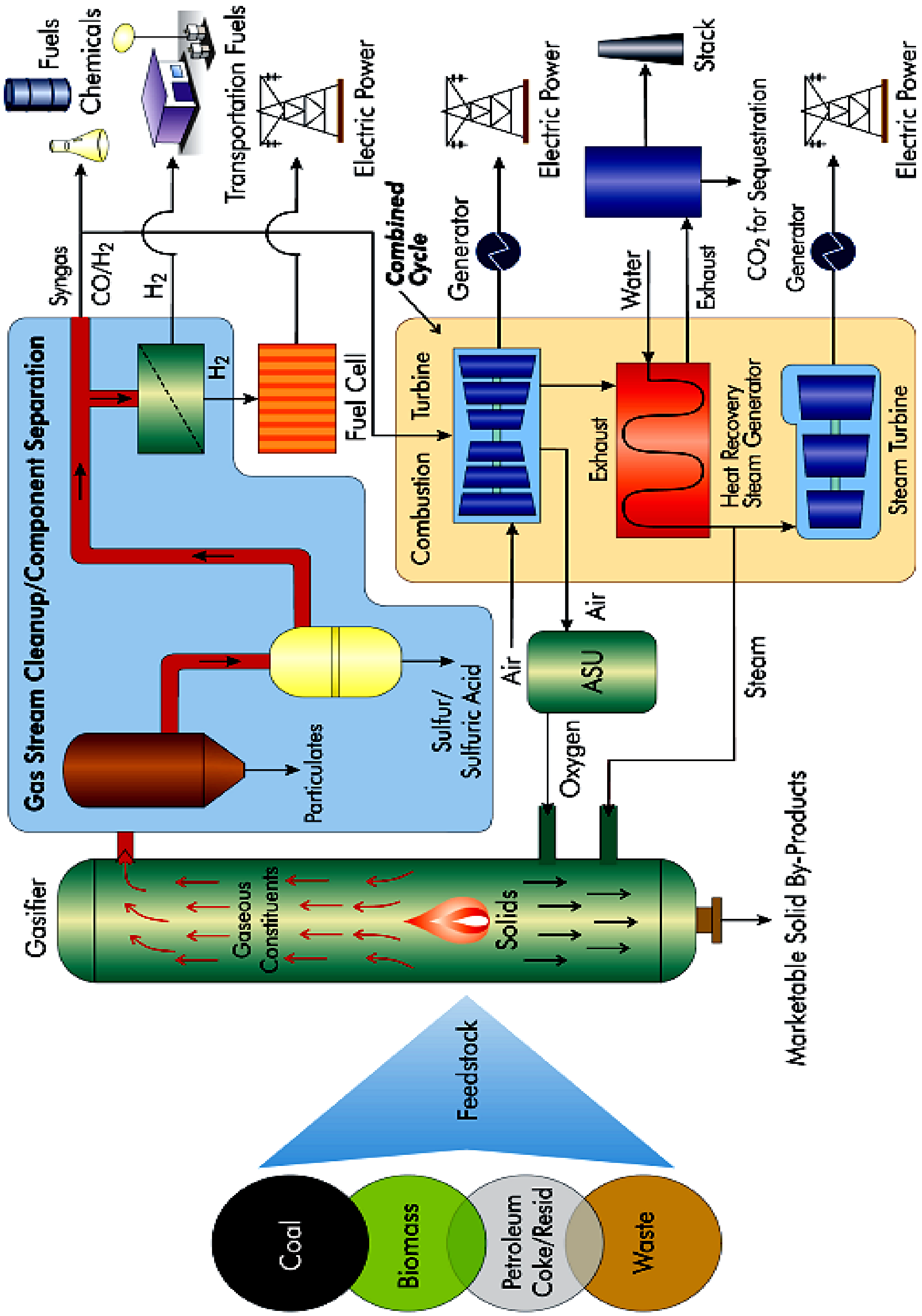

Fig. 3.2: Gasification Process: A Complete Scenario [2]

3.1.2 Hydrogenation

In a gasification process the feedstock is hydrogenated. This means hydrogen is added to the system directly or indirectly or the feedstock is pyrolyzed to remove carbon to produce a product with a higher hydrogen-to-carbon ratio than the feedstock [4-6].

3.1.3 Stoichiometric Considerations:

Depending on the gasification process, reactions that take place in a gasifier include:

$$C + O_2 \rightarrow CO_2 \quad (1)$$

$$C + {}^{1}/_{2}O_2 \rightarrow CO \quad (2)$$

$$H_2 + 1/2O_2 \rightarrow H_2O \quad (3)$$

$$C + H_2O \rightarrow CO + H_2 \quad (4)$$

$$C + 2H_2O \rightarrow CO_2 + 2H_2 \quad (5)$$

$$C + CO_2 \rightarrow 2CO \quad (6)$$

$$C + 2H_2 \rightarrow CH_4 \quad (7)$$

$$CO + H_2O \rightarrow H_2 + CO_2 \quad (8)$$

$$CO + 3H_2 \rightarrow CH_4 + H_2O \quad (9)$$

$$C + H_2O \rightarrow {}^{1}/_{2}CH_4 + {}^{1}/_{2}CO_2 \quad (10)$$

Most of the oxygen injected into a gasifier, either as pure oxygen or air, is consumed in reactions (1) through (3) to provide the heat necessary to dry the solid fuel, break up chemical bonds, and raise the reactor temperature to drive gasification reactions (4) through (9). Reactions (4) and (5), which are known as water-gas reactions, are the principal gasification reactions, are endothermic, and favor high temperatures and low pressures. Reaction (6), the *Boudourd reaction,* is endothermic and is much slower than the combustion reaction (1) at the same temperature in the absence of a catalyst. Reaction (7), hydro-gasification, is very slow except at high pressures. Reaction (8), the *water-gas shift reaction,* can be important if H_2 production is desired. Optimum yield is obtained at low temperatures (up to 500°F) in the presence of a catalyst and pressure has no effect on increasing hydrogen yield. Reaction (9), the *methanation reaction,* proceeds very slowly at low temperatures in the absence of catalysts. Reaction (10) is relatively thermal neutral, suggesting that gasification could proceed with little heat input but methane formation is slow relative to reactions (4) and (5) unless catalyzed [7-8].

3.1.4 Comparison between GASIFICATION and COMBUSTION:

Gasification is not an incineration or combustion process. Rather, it is a conversion process that produces more valuable and useful products from carbonaceous material. Table 1 compares the general features of gasification and combustion technologies.

Both gasification and combustion processes convert carbonaceous material to gases. Gasification processes operate in the absence of oxygen or with a limited amount of oxygen, while combustion processes operate with excess oxygen [1, 9, 10].

Table 3.1: Comparison between Gasification and Combustion

FEATURES	GASIFICATION	COMBUSTION
1. Purpose	Creation of valuables, usable products from waste or lower value material	Generation of heat or destruction of waste
2. Process type	Thermal and chemical conversion using no or limited oxygen	Complete combustion using excess oxygen
3. Raw gas composition (Before gas cleanup)	H_2, CO, H_2S, NH_3 and particulates	CO_2, H_2O, SO_2, NOx and particulates
4. Gas cleanup	a. Syngas cleanup at atm to high pressure depending on the gasifier design b. Treated syngas used for chemical, fuels	a. Flue gas cleanup at atm pressure b. Treated flue gas is discharged to atmosphere c. Any sulfur in the

	or power generation c. Recovers sulfur species in the fuel as sulfur or sulfuric acid d. Clean flue gas primarily consist of CO and H_2	fuel is converted to Sox that must be removed using flue gas cleanup system, generating a waste that must be land filled d. Clean flue gas primarily consist of CO_2 and H_2O
5. Solid byproducts	Char or slag	Bottom ash
6. Ash/char or slag handling	a. Low temp process produce a char that can be solid as flue b. High temp processes produce a slag, a non-leachable, non-hazardous material suitable for use as construction material Fine particles are recycled to gasifier as well as valuable metals if any	Bottom ash and fly ash are collected, treated and disposed as hazardous waste in most cases
7. Temperature	$1300^{o}F$ - $2700^{o}F$	$1500^{o}F$ - $1800^{o}F$
8. Pressure	Atmospheric to high	Atmospheric

3.1.5 Advantages of Gasification over Combustion:

From an environmental standpoint, gasification offers several advantages over the combustion of solids, heavy oils, and carbonaceous industrial and domestic wastes.

One study by the U.S. Department of Energy on *The Wabash River Coal Gasification Repowering Project* [11] shows that repowering of conventional coal-fired utility systems with IGCC systems can reduce sulfur and nitrogen oxides as well as particulate emissions by one to two orders of magnitude [12].

3.2 COAL GASIFICATION TECHNOLOGIES [1, 2]

Gasification can be thought of as a combustion process in which sufficient air is supplied to allow a portion of the carbonaceous feed material to burn. The heat that is generated is used to de-volatize and decompose majority of the remaining feed material into hydrocarbon gases. Gasification can be carried out in many different reactor types including:

- Fixed Bed
- Fluid Bed
- Bubbling, Circulating, Entrained, Twin Bed
- Moving Bed
- Rotary Kiln
- Cyclonic

Each of these technologies is discussed to the point of providing a working knowledge of the process, along with the advantages and disadvantages of each. Before discussing the processes, the chapter begins with an overview of coal gasification and the properties of coal that should be considered when evaluating the suitability of gasification for an application.

3.2.1 COAL GASIFICATION: OVERVIEW

Coal gasification is a process that converts coal from a solid to a gaseous fuel through partial oxidation. Once the fuel is in the gaseous state, undesirable substances, such as sulfur compounds and coal ash, may be removed from the gas. The net result is a clean, transportable gaseous energy source.

In contrast to combustion process, which works with excess air, the gasification process works on partial combustion of coal with the oxygen supply controlled (generally 20 to 70% of the amount of O_2 theoretically required for complete combustion) such that both heat and a new gaseous fuel are produced as the coal is consumed. In simplest terms, the stoichiometric reactions are as follows:

$$C + 1/2\ O_2 \rightarrow CO$$

$$C + H_2O \rightarrow CO + H_2$$

3.2.2 Types of Coal

There are several different types of coal, each displaying different properties resulting from their age and the depth to which they have been buried under other rocks. In some parts of the world (e.g. New Zealand), coal development is accelerated by volcanic heat or crustal stresses. The degree of coal development is referred to as a "rank" of coal with peat having the lowest rank and anthracite the highest [13].

The various types of coals are as follows:

3.2.2.1 Peat: Peat is the layer of vegetable material directly underlying the growing zone of a coal-forming environment. The vegetable material shows very little alteration and contains the roots of living plants. Peat is widely used as a domestic fuel in rural parts of the world.

3.2.2.2 Lignite: Lignite is geologically very young (upward of around 40,000 years). It is brown and can be soft and fibrous, containing discernible plant material. It also contains large amounts of moisture (typically around 70%) and hence, it has low energy content (around 8 to 10 MJ/kg). As the coal develops it loses its fibrous character and darkens in color.

3.2.2.3 Black coal: Black coal ranges from Cretaceous age (65 to 105 million years ago) to mid-Permian age (up to 260 million years ago). They are all black; some are sooty and still quite high in moisture (sub-bituminous coal). A common name for this coal in many parts of the world is "black lignite."

3.2.2.4 Anthracite: Anthracite is a hard, black, shiny form of coal that contains virtually no moisture and very low volatile content. Because of this, it burns with little or no smoke and is sold as a "smokeless fuel" [13].

3.2.3 Characteristics [3-4]

The characteristics of coals that determine classification and suitability for given applications are the proportions of volatile matter, fixed carbon, moisture, sulfur, and ash. Each of these is reported in the proximate analysis. Coal analyses can be reported on several bases: as-received, moisture-free (or dry), and mineral-matter-free (or ash-free). Heating values may be reported on an as-received, dry, dry and mineral-matter-free, or moist and mineral-matter free basis. Higher heating values of coals are frequently reported with their proximate analysis. The details are provided in table 3.2.

Table 3.2: Composition of different types of coal

Rank	**Calorific Value, Btu/lb**	**Percentage by mass**					
		C	**H**	**O**	**N**	**S**	**Ash**
Anthracite	12700	80	2.9	5	0.9	0.7	10.5
Semi-anthracite	13600	80.4	3.9	5	1.1	1.1	8.5
Low-volatile Bituminous	14350	81.7	4.7	5	9.4	1.2	6
High-volatile Bituminous A	13800	75.9	5.3	9.3	1.5	1.5	6.5
High-volatile Bituminous B	12500	67.8	5.5	13.8	1.4	3	8.5
High-volatile Bituminous C	11000	59.6	5.8	20.6	1.1	3.5	9.4
Sub-Bituminous B	9000	52.5	6.2	29.5	1	1	9.8
Lignite	6900	40.1	6.9	44	0.7	1	7.3

3.3 GASIFIER CONFIGURATIONS

3.3.1 Gasifier Classifications

Coal gasification technologies can be classified according to the flow configuration of the gasifier unit. The primary configurations are [14-15]:

- Entrained flow
- Fluidized bed
- Moving bed

A detailed comparison of these three types of beds is presented in table 3.3.

Table 3.3: Comparison of different types of gasifier beds

Parameters	**Fixed/moving Bed**	**Fluidized Bed**	**Entrained Bed**
Feed size	<51mm	<6mm	<0.15mm
Tolerance for fines	Limited	Good	Excellent
Tolerance for coarse	Very good	Good	Poor
Exit gas temp	450-650^{o}C	800-1000^{o}C	>1900^{o}C
Feed stock tolerance	Low rank coal	Low rank coal and excellent for biomass	Any coal including caking but unsuitable for biomass
Oxidant requirements	Low	Moderate	High
Reaction zone temp	1090^{o}C	800-1000^{o}C	>1990^{o}C
Steam requirement	High	Moderate	Low
Nature of ash produced	Dry	Dry	Slagging
Cold gas efficiency	80%	89.2%	80%
Application	Small capacities	Medium size capacities	Large capacities
Problem area	Tar production	Carbon conversion	Raw gas cooling

3.4 FLUIDIZATION [9]

The fluidized-bed reactor has the ability to process large volumes of fluid. For the catalytic cracking of petroleum naphtha to form gasoline blends, for example, the virtues of the fluidized-bed reactor drove its competitors from the market. The material “fluidized” is almost always a solid and the “fluidizing medium” is either a liquid or gas. The characteristics and behavior of a fluidized bed are strongly dependent on both the solid and liquid or gas properties [16-17].

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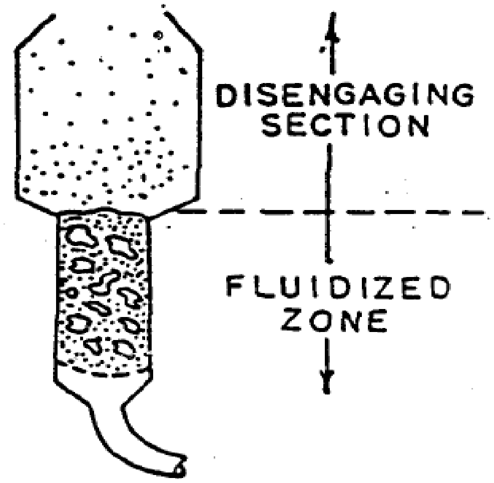


Fig. 3.3: Fluidized column zones

3.4.1 Operation of the Fluidized Bed Gasifier

Fluidized-bed gasifier employs back-mixing, and efficiently mix feed coal particles with coal articles already undergoing gasification. To sustain fluidization, or suspension of coal particles within the gasifier, coal of small particles sizes (<6 mm) is normally used. Coal enters at the side of the reactor, while steam and oxidant enter near the bottom with enough velocity to fully suspend or fluidize the reactor bed. This, in turn means that fluidized-bed gasifier are best suited to relatively reactive coals and other fuels such as biomass [18-19].

3.4.2 Characteristics [20, 21]

Fluidized-bed gasifies may differ in ash conditions (dry or agglomerated/ slagging) and in design configurations for improving char use. Also, depending on the degree of fluidization and bed height, these types of reactors sometimes are also named as circulating fluidized bed reactors, and/or transport reactors.

3.4.3 ADVANTAGES OF FLUIDIZED BED GASIFICATION [22]

- Air to fuel ratio can changed which also helps to control the bed temperature.

- Fluidized bed gasifiers are more tolerant to variation in feedstock as compared to other types of gasifiers.
- They maintain uniform radial temperature profiles and avoid slagging problems.
- Higher throughput of fuel as compared to other gasifiers.
- Improved mass and heat transfer from fuel.
- High heating value.
- Reduced char.

3.4.4 DISADVANTAGES OF FLUIDIZED BED GASIFICATION

- Oxidizing conditions are created when oxygen diffuses from bubble to the emulsion phase thereby reducing the gasification efficiency.
- Reduced solid conversion due to intimate mixing of fully and partially gasified fuels.
- Losses occurring due to particle entrainment.

3.5 MATERIAL AND ENERGY BALANCE

To develop the model, the chemical formula of feedstock is defined as $CH_xO_yN_z$. The global gasification reaction can be written as follows:

$$\mathbf{CH_xO_yN_z + wH_2O + m(O_2 + 3.76N_2) = n_{H2}H_2 + n_{CO}CO + n_{CO2}CO_2 + n_{H2O}H_2O + n_{CH4}CH_4 + (z/2 + 3.76m)N_2} \quad (1)$$

where x, y, and z are the number of atoms of hydrogen, oxygen, and nitrogen per number of atom of carbon in the feedstock, respectively; w is the amount of moisture per kmol of feedstock; and m is the amount of oxygen per kmol of feedstock. All inputs on the left-hand side of equation (1) are defined at 25^0C. On the right-hand side, n_i are the numbers of mole of the species i that are also unknown.

3.5.1 Mass balance

To find the five unknown species of the producer gas, five equations were required. Those equations were generated using mass balance and equilibrium constant relationships. Considering the global gasification reaction in equation (1), the first three equations were formulated by balancing each chemical element as shown in equations (2–4).

Carbon balance:

$$f_1 = 0 = n_{CO} + n_{CO2} + n_{CH4} - 1 \qquad (2)$$

Hydrogen balance:

$$f_2 = 0 = 2n_{H2} + 2n_{H2O} + 4n_{CH4} - x - 2w \qquad (3)$$

Oxygen balance:

$$f_3 = 0 = n_{CO} + 2n_{CO2} + n_{H2O} - w - 2m - y \qquad (4)$$

3.5.2 Thermodynamic equilibrium [13, 23-25]

Chemical equilibrium is usually explained either by minimization of Gibbs free energy or by using an equilibrium constant. To minimize the Gibbs free energy, constrained optimization methods are generally used which requires an understanding of complex mathematical theories. For that reason, the present thermodynamic equilibrium model is developed based on the equilibrium constant and not on the Gibbs free energy. The remaining two equations were obtained from the equilibrium constant of the reactions occurring in the gasification zone as shown below:

Boudouard reaction: $C + CO_2 = 2CO$ (5)

Water-gas reaction: $C + H_2O = CO + H_2$ (6)

Methane reaction: $C + 2H_2 = CH_4$ (7)

Equations (5) and (6) can be combined to give the water–gas shift reaction by subtracting equation (5) from (6).

Water-gas shift reaction:

$$CO_2 + H_2O = CO_2 + H_2 \qquad (8)$$

For the model in this study, the thermodynamic equilibrium was assumed for all chemical reactions in the gasification zone. All gases were assumed to be ideal and all reactions form at pressure 1 atm. Therefore, the equilibrium constants, which are functions of temperature for the water–gas shift reaction and the methane reaction, are [4, 9]:

The equilibrium constant for water–gas shift reaction

$$K_1 = \frac{(n_{CO\,2})(n_{H\,2})}{(n_{CO})(n_{H\,2O})} \qquad (9)$$

The equilibrium constant for methane reaction

$$K_2 = \frac{(n_{CH\,4})}{(n_{H\,2})2} \qquad (10)$$

where x_i is mole fraction of species i in the ideal gas mixture, n is stoichiometric number (positive value for products and negative value for reactants), P^o is standard pressure, 1 atm. Equations (9) and (10) can be modified as:

$$f_4 = 0 = K_1\,(n_{CO})\,(n_{H2O}) - (n_{CO2})\,(n_{H2}) \qquad (11)$$

$$f_5 = 0 = K_2\,(n_{H2})^2 - (n_{CH4}) \qquad (12)$$

Equations (13) and (14) were used for the equilibrium state of ideal gas mixture because of the requirements of K_1 and K_2 values.

$$\ln K = -\frac{\Delta G_T^0}{RT} \qquad (13)$$

$$\Delta G_T^0 = \sum_i \; vi\Delta\bar{g}_{f,T,i}^0 \qquad (14)$$

where R is the universal gas constant, 8.314 kJ/(kmol.K), ΔG_T^0 is the standard Gibbs function of reaction, and $\Delta\bar{g}_{f,T,i}^0$ represents the standard Gibbs function of formation at given temperature T of the gas species i which can be expressed by the empirical equation below [26]:

$$\Delta\bar{g}_{f,T,}^0 = \overline{h_f^0} - a'Tln(T) - b'T^2 - \left(\frac{c'}{2}\right)T^3 - \left(\frac{d'}{3}\right)T^4 + \left(\frac{e'}{2T}\right) + f' + g' \qquad (15)$$

Table 3.4 shows the thermodynamic conditions used for analysis. The values of coefficients a'–g' and the enthalpy of formation of the gases are presented in table 3.5. For calculating K_1 and K_2, the temperature in the gasification or reduction zone must be known. In this study, it was determined using energy balance method as explained in section 4.3.

With Coal having ($C_1H_{0.872}O_{0.285}$) molecular structure, calculations were carried out and the results are tabulated.

Table 3.4: Thermodynamic conditions for analysis

P (bar)	T (K)	Hf^0 (kJ/kg)	Hf^0(kJ/kmol)
20	700	3917	217.6111111

Table 3.5: Calculation of coefficients for determining Gibbs free energy [27]

Compound	**h_f^0**	**a'**	**b'**	**c'**	**d'**	**e'**	**f'**	**g'**
CO	**-110.5**	**0.005619**	**-0.0000119**	**6.383 E-09**	**-1.846 E-12**	**-489.1**	**0.8684**	**-0.06131**
CO_2	**-393.5**	**-0.01949**	**3.1225E-05**	**-2.45 E-08**	**6.946 E-12**	**-489.1**	**5.27**	**-0.1207**
H_2O	**-241.8**	**-0.00895**	**-3.672E-06**	**5.209 E-09**	**-1.478 E-12**	**0**	**2.868**	**-0.01722**
CH_4	**-74.8**	**-0.0462**	**0.0000113**	**1.319 E-08**	**-6.647 E-12**	**-489.1**	**14.11**	**-0.2234**

LHV= HHV-22604H-2581M

HHV(kJ/kg) = 33823*C+144249*(H-(O/8))+9418*S

HHV(kJ/kg) = 25758.51925

LHV(kJ/kg) = 24628.31925

$H_{f\ coal}^{0}$= (LHV/MW of COAL)+$\sum(Hf_0CO2+Hf_0H2O)$

$H_{f\ coal}^{0}$= -497511.9776 kJ/kg

3.5.3 Energy balance

The temperature of the gasification zone needs to be calculated in order to calculate the equilibrium constants (equations 13–15). For this reason, either energy or enthalpy balance was performed for the gasification process which was usually assumed to be an adiabatic process. When the temperature in gasification zone is T and the temperature at inlet state is assumed to be 298 K (25^{o}C), the enthalpy balance for this process can be written as:

$$\sum_{j=react} \bar{h}^{0}_{f,j} = \sum_{i=prod} ni(\bar{h}^{0}_{f,i} + \Delta\bar{h}^{0}_{T,i}) \qquad (16)$$

where $\bar{h}^{0}_{f}$ is the enthalpy of formation in kJ/kmol and its value is zero for all chemical elements at reference state (298 K, 1 atm), and $\Delta\bar{h}_{T}$ represents the enthalpy difference between any given state and at reference state. It can be approximated by

$$\Delta\bar{h}_{T} = \int_{298}^{T} \bar{C}_{p}(T)dT \qquad (17)$$

where $\bar{C}_{p}(T)$ is specific heat at constant pressure in kJ/kmolK and is a function of temperature. It can be defined by the empirical equation below:

$$\bar{C}_{p}(T) = a + bT + cT^{2} + dT^{3} \qquad (18)$$

where T is the temperature in K and

$$\int_{298}^{T} \bar{C}_{p}(T)dT = aT + bT^{2} + cT^{3} + dT^{4} \qquad (19)$$

Where k is a constant obtained from the integration and a, b, c, and d are the specific gas species coefficients, which are shown in table 3.6.

Table 3.6: Coefficients for specific heat calculations [23, 24]

Gas Species	a	b	c	d	Temp. range, K
Hydrogen	28.6105	0.0010194	-1.476E-07	7.69E-10	298-1500
CO	29.0277	-0.0028165	1.16437E-05	-4.7063E-09	298-1500
CO_2	21.3655	0.0642841	-4.10506E-05	9.7999E-09	298-1500
Water Vapour	32240	1.923	0.01055	-0.000003595	298-1500
CH_4	19.2494	0.0521135	0.000011973	-1.13173E-08	298-1500
N_2	29.5909	-0.005141	1.31829E-05	-4.968E-09	298-1500

Equation (16) can be rewritten as:

$$\sum_{j=react} \bar{h}^0_{f,j} = \sum_{i=prod} ni\bar{h}^0_{f,i} + [(\sum_i niai)T + (\sum_i nibi)T^2 + (\sum_i nici)T^3 + inidiT4 \tag{20}$$

De Souza-Santos [4] suggested the relationship for finding the enthalpy of formation for solid fuel in reactant that is:

$$\bar{h}^0_{f,fuel} = \overline{LHV} + \sum_{k=prod} \left[n_k \left(\bar{h}^0_f\right)_k\right] \tag{21}$$

where $\left(\bar{h}^0_f\right)_k$ is the enthalpy of formation of product k under complete combustion of the solid fuel and $\overline{LHV}$ is the lower heating value of the solid fuel in kJ/kmol. Now that the enthalpies of formation in equation (16) can be solved, the temperature in the gasification zone can finally be calculated from equation (20) The Gibbs energy change for compounds are indicated in tables 3.7 and 3.8.

Table 3.7: Gibbs free energy overall calculations

Compound	**a'T*lnT**	**b'T*T**	**0.5*c'*t^3**	**0.33*d'*T^4**	**(0.5*e')/T**	**g'*T**	**Δg**
CO	61.639478	-26.775	10.7713	-3.08397375	-0.163033	-91.965	-244311.4501
CO_2	-213.802	70.25625	-41.31	11.60416125	-0.163033	-181.05	-396191.4466
H_2O	-98.179984	-8.262	8.7901	-2.46918375	0	-25.83	-164641.0201
CH_4	-506.80617	25.425	22.258	-11.10464438	-0.163033	-335.1	74274.65887

Separate calculations are performed for following two reactions.

$$CO + H_2O = CO_2 + H_2$$

$$C + 2H_2 = CH_4$$

The above two reactions are chosen as they help in enhancing the H_2/CO, which in turn enhances the quality of the synthesis gas being produced.

Table 3.8: Gibbs free energy calculations for two specific reactions

compound	**h_f^0**	**a'**	**b'**	**c'**	**d'**	**e'**	**f'**	**g'**
CO	-110.5	0.005619	-1.19E-05	6.383E-09	-1.846E-12	-489.1	0.8684	-0.06131
CO_2	-393.5	-0.01949	3.123E-05	-2.45E-08	6.946E-12	-489.1	5.27	-0.1207
H_2O	-241.8	-0.00895	-3.67E-06	5.209E-09	-1.478E-12	0	2.868	-0.01722
CH_4	-74.8	-0.0462	0.0000113	1.319E-08	-6.647E-12	-489.1	14.11	-0.2234

The overall results are provided in table 3.9.

Table 3.9: Gibbs energy and equilibrium constants

ΔG^o_{T1}	ΔG^o_{T2}	$\ln K_1$	$\ln K_2$	**$K1_{1500K}$**	**$K2_{1500K}$**
12761.02	74274.65887	-1.023	-5.9558	**0.359423**	**0.00259**

Enthalpy of product at standard conditions $\sum N_i H_{fi}$= -582045

Heat capacity coefficients are calculated for four compounds and are tabulated in table 3.10.

Table 3.10: Heat capacity coefficients

$\sum n_i a_i$	$0.5^*\sum n_i b_i$	$0.33^*\sum n_i c_i$	$0.25^*\sum n_i d_i$
48935.80181	24467.90091	16148.8146	12233.95045

$$H_f^o \text{ REACTANT} = H_f^o \text{ PRODUCT} + \Delta h_T \text{ PRODUCT}$$

$$\Delta h_T \text{ PRODUCT} = H_f^o \text{ REACTANT} - H_f^o \text{ PRODUCT}$$

$$\Delta h_T \text{ PRODUCT} = 30996.37008$$

To determine the optimum H_2/CO ratio that can be generated using above thermodynamic data, we developed a MATLAB code in MathWorks' MATLAB ®. Using the code, we could generate the best possible ratio, providing us much better quality of Synthesis Gas than being produced with non optimized fluidized bed gasifiers at present. The code and the results are produced below.

3.5.4 Coding using Mathworks' MATLAB®:

MATLAB CODE

```
function x = Ratnadip_mulNR(x)
a = x(1);
b = x(2);
c = x(3);
d = x(4);
e = x(5);
i = 1;
for i =1:10
df1dx1 = 1;
df1dx2 = 1;
df1dx3 = 1;
df1dx4 = 0;
df1dx5 = 0;
df2dx1 = 0;
df2dx2 = 0;
df2dx3 = 4;
df2dx4 = 2;
df2dx5 = 2;
df3dx1 = 1;
df3dx2 = 2;
df3dx3 = 0;
df3dx4 = 0;
df3dx5 = 1;
df4dx1 = .359423*e;
df4dx2 = - d;
df4dx3 = 0;
```

```
df4dx4 = - b;
df4dx5 = .359423*a;
df5dx1 = 0;
df5dx2 = 0;
df5dx3 = - 1;
df5dx4 = (2*.00259*d);
df5dx5 = 0;
A = [df1dx1 df1dx2 df1dx3 df1dx4 df1dx5; df2dx1 df2dx2 df2dx3 df2dx4 df2dx5;
...
df3dx1 df3dx2 df3dx3 df3dx4 df3dx5; df4dx1 df4dx2 df4dx3 df4dx4 df4dx5;
...
df5dx1 df5dx2 df5dx3 df5dx4 df5dx5];
f1 = a+b+c-1;
f2 = 2*d+2*e+4*c-4.872;
f3 = a+(2*b)+e-2.885;
f4 = .359423*(a*e) - (b*d);
f5 = .00259*(d^2) - c;
F = [f1; f2; f3; f4; f5]
xnew = x - (inv(A)*F);
eps = x - xnew;
x = xnew
a = x(1);
b = x(2);
c = x(3);
d = x(4);
e = x(5);
i = i+1;
End
```

Table 3.11: MATLAB Solution

Compound	No. of moles by using MATLAB
n-CO	0.6259
n-CO_2	0.3719
n-CH_4	0.0022
n-H_2	0.9164
n-H_2O	1.5152
n-N_2	1.128

While many of fluidized bed gasifiers are providing H_2/CO ration ranging from 0.6 to 1.2, our present calculations show accomplishment of 1.46 or approximately 1.5 as the final ratio. This is an outcome of the present study. At present, many attempts [28] are being made to enhance this ratio to overcome high CO and CO_2 formation by gasification of coal as well as wood [29]. The detailed thermodynamic analysis and precise modeling of the gasification process in the present study has raised this ratio from 0.6 at underground coal gasification [11] to present accomplishment of approximately 1.5 in this work.

Using these data and H_2/CO ratio, now we have designed the fluidized bed reactor. After process design, the hydrodynamic calculations are performed as provided below.

3.6 DESIGN CALCULATIONS

3.6.1 Fluidization velocity

3.6.1.1 Terminology:

Minimum fluidization velocity: The lower limit of the superficial velocity of the gas that will flow through the particle bed was calculated separately for the sand and the rice husk using the expression in equation (22) [9, 10, 14, 17]:

$$U_{mf} = \frac{dp^{2}.(\rho_p - \rho_f).g}{150.\mu} X \frac{\varepsilon^{3}.\varphi^{2}}{1-\varepsilon} \tag{22}$$

Terminal velocity of the particle: The maximum value of the superficial velocity of the gas was determined for both materials of the bed depending of the Reynolds number (for 0.4 < Re < 50) of the particle [2]:

$$U_{t=} d_p \left[\frac{4.(\rho_p - \rho_f)^{2}.g^{2}}{225.\rho_f.\mu}\right]^{\frac{1}{3}} \tag{23}$$

Fluidization velocity during the gasification: The superficial velocity of the gas to be used during the gasifier operation was established considering the relation between the expanded and minimum heights of the fluidized bed [14]:

$$\frac{H}{H_{mf}} = 1 + \frac{10.978.(U_f - U_{mf})^{0.738}.\rho_p{}^{0.376}.d_p{}^{1.006}}{U_{mf}{}^{0.937}.\rho_f{}^{0.126}} \tag{24}$$

For the bubbling fluidized bed the restriction suggested in equation (25) was used [9]:

$$1.2 < \frac{H}{H_{mf}} < 1.4 \tag{25}$$

For the design, a value of 1.3 was selected for the equation (25), and the equation (24) was solved to determine the value of U_f.

$$H_t = TDH + H$$

Table 3.12: Carbon composition and density of various coal samples used [1]

Type of coal	% of 'C' in coal	ρ_p (kg/m$^{3)}$
Lignite	0.4	753
High Volatile Bituminous B	0.67	793
Anthracite	0.8	865

3.6.1.2 Calculations for minimum fluidization velocity:

$$U_{mf} = \frac{dp^2.(\rho_p - \rho_f).g}{150.\mu} X \frac{\varepsilon^3.\varphi^2}{1-\varepsilon}$$

Using g =9.81m^2/s

Table 3.13: Various parameters for coal samples selected

dp (m)	**Φ**	**ρ_p (kg/m$^{3)}$**	**ρ_f (kg/m^3)**	**ε_{mf}**	**μ (kg/ms)**
0.0005	**0.63**	**753**	**0.28**	**0.503**	**0.000039**
0.0005	**0.63**	**793**	**0.28**	**0.503**	**0.000039**
0.0005	**0.63**	**865**	**0.28**	**0.503**	**0.000039**

Calculation for $\boldsymbol{\varepsilon_{mf}}$ [9]:

$$\varepsilon_{mf} = 0.768-0.42*\Phi$$

U_{mf} values obtained from above data:

Table 3.14: Minimum fluidization velocities for coal samples selected

Type of coal	u_{mf} (m/s)
Lignite	0.0983
High Volatile Bituminous B	0.1035
Anthracite	0.1129

3.6.1.3 Calculation for fluidization velocity at Gasification:

Assuming: $1.2 < \frac{H}{H_{mf}} < 1.4$

$$\frac{H}{H_{mf}} = 1.3$$

Calculating U_f from following equation:

$$\frac{H}{H_{mf}} = 1 + \frac{10.978.(U_f - U_{mf})^{0.738}.\rho_p{}^{0.376}.d_p{}^{1.006}}{U_{mf}{}^{0.937}.\rho_f{}^{0.126}}$$

Taking data from U_{mf} and above table, U_f is calculated.

Table 3.15: Fluidization velocity at gasification for coal samples selected

Type of coal	u_f (m/s)
Lignite	0.447
High Volatile Bituminous B	0.466
Anthracite	0.5

3.6.1.4 Calculating terminal fluidization velocity, U_t :

$$U_{t=}d_p\left[\frac{4.(\rho_p - \rho_f)^2.g^2}{225.\rho_f.\mu}\right]^{\frac{1}{3}}$$

Table 3.16: Terminal fluidization velocity for coal samples selected

Type of coal	U_t (m/s)
Lignite	2.23
High Volatile Bituminous B	2.309
Anthracite	2.447

3.6.2 MATERIAL BALANCE

Table 3.17: Composition of coal samples for material balance calculations

Coal Samples for study	Composition of coal/gram		
	C	Ash	Others
Lignite	0.8	0.15	0.05
High volatile Bituminous B	0.4	0.4	0.2
Anthracite	0.67	0.3	0.03

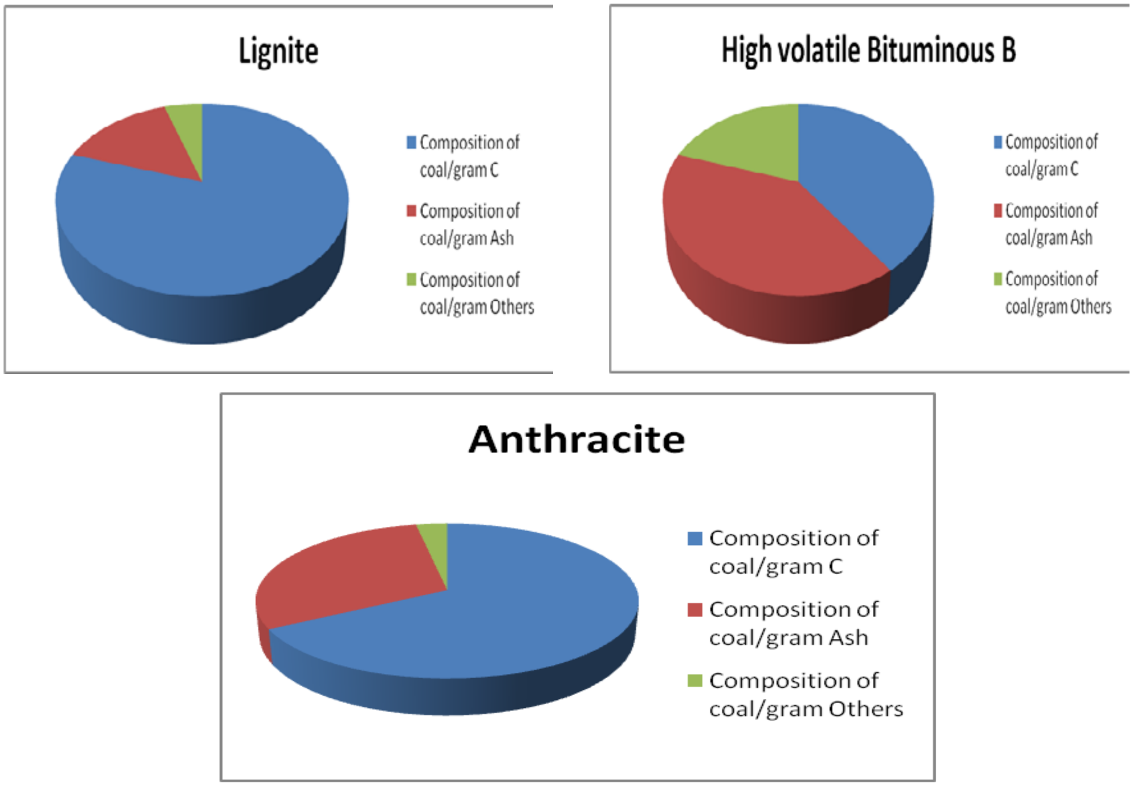


Fig. 3.4: Composition of coal samples selected for calculations

3.6.2.1 Reactions considered for material balance calculations:

$$C + H_2O \longrightarrow CO + H_2$$

$$CO + 0.5\ O_2 \longrightarrow CO_2$$

3.6.2.2 Assumptions:

CO to CO_2 conversion = 20%

Specific volume of saturated steam =0.09409 m^3/ kmol

Calculations are performed for three mass flowrates of coal, as 1000 kg/hr, 700 kg/hr and 360 kg/hr. The bases are chosen as per requirement of synthesis gas for various purposes. This serves the need of medium to large plants for production of quality synthesis gas for power as well as production of chemicals.

BASIS: 1000 kg/hr

Table 3.18: Stoichiometric balance for the reactions

Available moles of reactants, kmol		**Required moles, kmol**		
C	**CO**	**CO_2**	**O_2**	**H_2O**
33.33	33.33	6.66	3.33	33.33
55.83	55.83	11.16	5.58	55.83
66.66	66.66	13.33	6.66	66.66

Table 3.19: Required flowrate of utilities

O_2 (Nm^3/hr)	**H_2O, (Nm^3/hr) (Saturated Steam)**	**Total flowrate, (Nm^3/hr)**	**Total flowrate (Nm^3/s)**
74.66	3.13	77.80	0.021
125.06	5.25	130.32	0.036
149.33	6.27	155.60	0.043

BASIS: 700 kg/hr

Table 3.20: Stoichiometric balance for the reactions

Available moles of reactants, kmol		**Required moles, kmol**		
C	**CO**	**CO_2**	**O_2**	**H_2O**
39.08	39.08	7.81	3.90	39.08
46.66	46.66	9.33	4.66	46.66
23.33	23.33	4.66	2.33	23.33

Table 3.21: Required flowrate of utilities

O_2 (Nm^3/hr)	H_2O, (Nm^3/hr) (Saturated Steam)	Total flowrate, (Nm^3/hr)	Total flowrate (Nm^3/s)
87.54	3.67	91.22	0.025
104.53	4.39	108.92	0.030
52.26	2.19	54.46	0.015

BASIS: 360 kg/hr

Table 3.22: Stoichiometric balance for the reactions

Available moles of reactants, kmol		Required moles, kmol		
C	CO	CO_2	O_2	H_2O
20.1	20.1	4.02	2.01	20.1
24	24	4.8	2.4	24
12	12	2.4	1.2	12

Table 3.23: Required flowrate of utilities

O_2 (Nm^3/hr)	H_2O, (Nm^3/hr) (Saturated Steam)	Total flowrate, (Nm^3/hr)	Total flowrate (Nm^3/s)
45.024	1.89	46.91	0.013
53.76	2.25	56.01	0.015
26.88	1.129	28.00	0.007

Assuming ε = 0.65 to calculate superficial velocity U_t from figure 3.5 [9]:

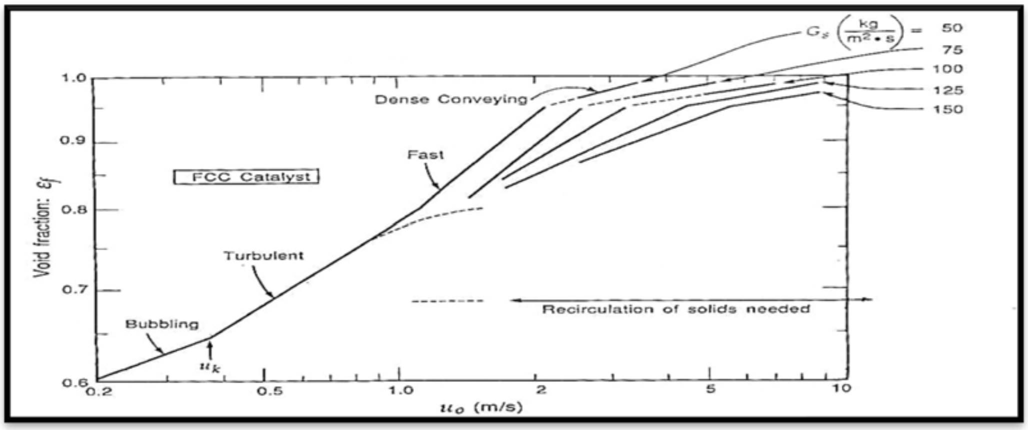


Fig. 3.5: Calculation of Superficial Velocity U_o [9]

From graph, we get U_o as 0.45 m/s

Assuming internal diameter of bed 0.5m, we calculate cross section area of bed.

$$A= (\pi/4)*d_t^2$$

Sample calculations for determination of parameters such as cross sectional area, Q, $H_{mf,}$ H, TDH, H_t are presented below. The detailed voluminous calculations for nine processes, as three samples for three different flowrates, are presented in tables 3.25 through 3.33.

Sample calculation:

For d_t = 0.5 m, A = 0.19625 m^2

From table 3.15, we fetch the values of U_f and calculate the volumetric flowrate of excess steam required (Qex) to fluidize the bed using Q=A * U

Sample calculation:

For U_f = 0.466 m/s,

Qex = 0.466 * 0.19625

Qex= 0.08765 m^3/s

3.6.2.3 Volumetric flowrate calculations:

Sample calculations:

Dividing the basis taken as 1000 kg/hr by coal density of one of the sample, we get:

$$Q= 1000/753$$

$$Q=1.32\ m^3/hr$$

For Volumetric flowrate at minimum fluidization velocity, we divide the volumetric flowrate by bed porosity.

Sample calculations:

$$Q_{mf}=1.32/0.503$$

$$Q_{mf} =2.64\ m^3/hr$$

3.6.2.4 Calculation of height at minimum fluidization H_{mf}

Dividing the above calculated value by cross sectional area for one hour of operations, we get H_{mf}:

<u>Sample calculations:</u>

H_{mf} = 2.64/ 0.19625

H_{mf} = 13.453

We use the assumption $\frac{H}{H_{mf}} = 1.3$ and calculate H as given below:

H =1.3*13.453

H =17.489 m

Then from dt, we calculate TDH (transport disengaging height)/dt from figure 3.6 using Uo as 0.45:

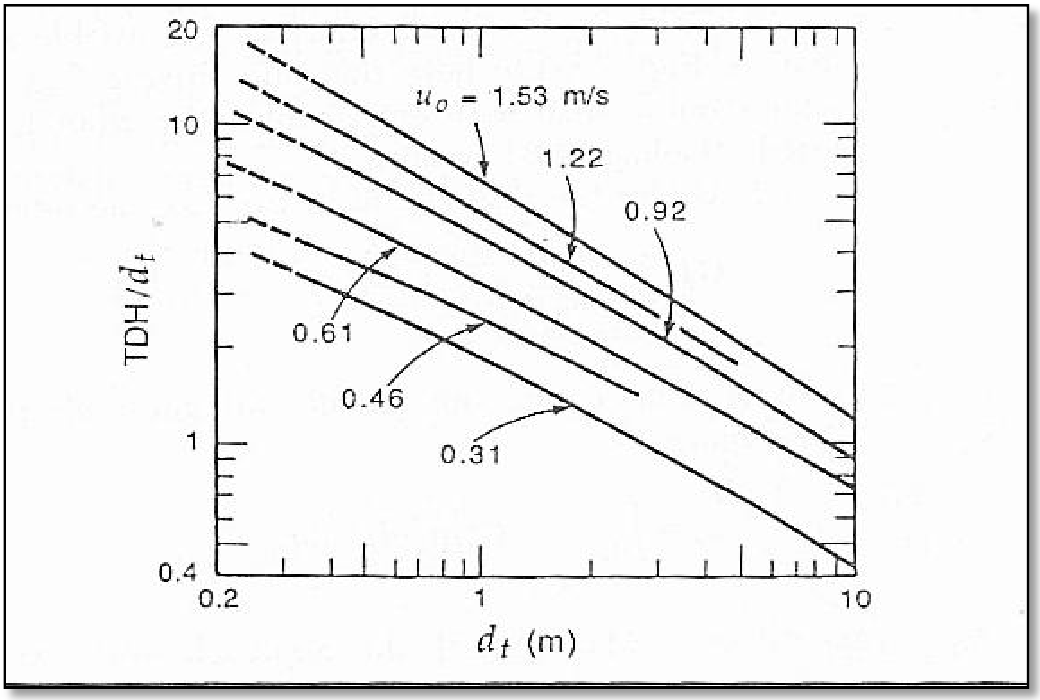


Fig. 3.6: Zens And Weil Correlations for TDH calculation [9]

Calculation of total height of bed H_t:

$$H_t = TDH + H$$

<u>Sample calculations:</u> H_t= 1.75+17.48

H_t = 19.23 m

Similarly, various diameters are assumed to calculate total height of gasifier. The diameters chosen are as following:

Table 3.24: Selection of various diameters for gasifier design

Sl. No.	Diameter, m	Sl. No.	Diameter, m
1	0.5	5	2.5
2	1.0	6	3.0
3	1.5	7	3.5
4	2.0	8	4.0

Calculating cross sectional area, Q, $H_{mf,}$ H, TDH, H_t for different flow rates as 1000 kg/hr, 700 kg/hr, 360 kg/hr for three different coal samples at different fluidization velocities are presented below in tables 3.25 through 3.33.

Table 3.25: Calculation of gasifier height for 1000 kg/hr at U_f = 0.4466

Basis mass flow rate: 1000 kg/hr										
U_f = 0.4466										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**H_{mf}**	**H**	**TDH/dt**	**TDH**	**H_t**
0.5	0.19625	0.08765	0.10926	1.32802	2.6402	13.4533	17.4892	3.5	1.75	19.2392
0.5	0.19625	0.08765	0.12385	1.26103	2.50703	12.7747	16.6071	3.5	1.75	18.3571
0.5	0.19625	0.08765	0.13088	1.15607	2.29835	11.7113	15.2247	3.5	1.75	16.9747
1	0.785	0.35061	0.37222	1.32802	2.6402	3.36331	4.37231	2.2	2.2	6.57231
1	0.785	0.35061	0.38681	1.26103	2.50703	3.19366	4.15176	2.2	2.2	6.35176
1	0.785	0.35061	0.39383	1.15607	2.29835	2.92783	3.80618	2.2	2.2	6.00618
1.5	1.76625	0.78887	0.81048	1.32802	2.6402	1.49481	1.94325	2	3	4.94325
1.5	1.76625	0.78887	0.82507	1.26103	2.50703	1.41941	1.84523	2	3	4.84523

1.5	1.76625	0.78887	0.83209	1.15607	2.29835	1.30126	1.69164	2	3	4.69164
2	3.14	1.40243	1.42404	1.32802	2.6402	0.84083	1.09308	1.6	3.2	4.29308
2	3.14	1.40243	1.43863	1.26103	2.50703	0.79842	1.03794	1.6	3.2	4.23794
2	3.14	1.40243	1.44566	1.15607	2.29835	0.73196	0.95155	1.6	3.2	4.15155
2.5	4.90625	2.1913	2.21291	1.32802	2.6402	0.53813	0.69957	1.4	3.5	4.19957
2.5	4.90625	2.1913	2.2275	1.26103	2.50703	0.51099	0.66428	1.4	3.5	4.16428
2.5	4.90625	2.1913	2.23453	1.15607	2.29835	0.46845	0.60899	1.4	3.5	4.10899
3	7.065	3.15547	3.17709	1.32802	2.6402	0.3737	0.48581	1.2	3.6	4.08581
3	7.065	3.15547	3.19167	1.26103	2.50703	0.35485	0.46131	1.2	3.6	4.06131
3	7.065	3.15547	3.1987	1.15607	2.29835	0.32531	0.42291	1.2	3.6	4.02291
3.5	9.61625	4.29495	4.31656	1.32802	2.6402	0.27456	0.35692	1.1	3.85	4.20692
3.5	9.61625	4.29495	4.33115	1.26103	2.50703	0.26071	0.33892	1.1	3.85	4.18892
3.5	9.61625	4.29495	4.33817	1.15607	2.29835	0.23901	0.31071	1.1	3.85	4.16071
4	12.56	5.60973	5.63134	1.32802	2.6402	0.21021	0.27327	1	4	4.27327
4	12.56	5.60973	5.64593	1.26103	2.50703	0.1996	0.25949	1	4	4.25949
4	12.56	5.60973	5.65296	1.15607	2.29835	0.18299	0.23789	1	4	4.23789

Table 3.26: Calculation of gasifier height for 1000 kg/hr at $U_{f} = 0.4685$

Basis mass flow rate: 1000 kg/hr										
$U_{f} = 0.4685$										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.091422	0.113034	1.328021	2.640201	13.45325	17.48923	3.5	1.75	19.23923
0.5	0.19625	0.091422	0.127622	1.261034	2.507026	12.77465	16.60705	3.5	1.75	18.35705

0.5	0.19625	0.091422	0.134646	1.156069	2.298349	11.71133	15.22473	3.5	1.75	16.97473
1	0.785	0.365688	0.3873	1.328021	2.640201	3.363314	4.372308	2.2	2.2	6.572308
1	0.785	0.365688	0.401888	1.261034	2.507026	3.193664	4.151763	2.2	2.2	6.351763
1	0.785	0.365688	0.408912	1.156069	2.298349	2.927833	3.806182	2.2	2.2	6.006182
1.5	1.76625	0.822799	0.844411	1.328021	2.640201	1.494806	1.943248	2	3	4.943248
1.5	1.76625	0.822799	0.858999	1.261034	2.507026	1.419406	1.845228	2	3	4.845228
1.5	1.76625	0.822799	0.866023	1.156069	2.298349	1.301259	1.691637	2	3	4.691637
2	3.14	1.462753	1.484365	1.328021	2.640201	0.840828	1.093077	1.6	3.2	4.293077
2	3.14	1.462753	1.498953	1.261034	2.507026	0.798416	1.037941	1.6	3.2	4.237941
2	3.14	1.462753	1.505977	1.156069	2.298349	0.731958	0.951546	1.6	3.2	4.151546
2.5	4.90625	2.285551	2.307163	1.328021	2.640201	0.53813	0.699569	1.4	3.5	4.199569
2.5	4.90625	2.285551	2.321752	1.261034	2.507026	0.510986	0.664282	1.4	3.5	4.164282
2.5	4.90625	2.285551	2.328775	1.156069	2.298349	0.468453	0.608989	1.4	3.5	4.108989
3	7.065	3.291194	3.312806	1.328021	2.640201	0.373702	0.485812	1.2	3.6	4.085812
3	7.065	3.291194	3.327394	1.261034	2.507026	0.354852	0.461307	1.2	3.6	4.061307
3	7.065	3.291194	3.334418	1.156069	2.298349	0.325315	0.422909	1.2	3.6	4.022909
3.5	9.61625	4.479681	4.501293	1.328021	2.640201	0.274556	0.356923	1.1	3.85	4.206923
3.5	9.61625	4.479681	4.515881	1.261034	2.507026	0.260707	0.338919	1.1	3.85	4.188919
3.5	9.61625	4.479681	4.522905	1.156069	2.298349	0.239007	0.310709	1.1	3.85	4.160709
4	12.56	5.851012	5.872624	1.328021	2.640201	0.210207	0.273269	1	4	4.273269
4	12.56	5.851012	5.887212	1.261034	2.507026	0.199604	0.259485	1	4	4.259485
4	12.56	5.851012	5.894236	1.156069	2.298349	0.18299	0.237886	1	4	4.237886

Table 3.27: Calculation of gasifier height for 1000 kg/hr at $U_{f =}$ 0. 5

Basis mass flow rate: 1000 kg/hr										
U_f = 0.5										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.119738	0.098126	0.119738	1.328021	2.640201289	13.45325	17.48923	3.5	1.75	19.23923
0.5	0.134326	0.098126	0.134326	1.261034	2.50702594	12.77465	16.60705	3.5	1.75	18.35705
0.5	0.14135	0.098126	0.14135	1.156069	2.298348637	11.71133	15.22473	3.5	1.75	16.97473
1	0.414117	0.392505	0.414117	1.328021	2.640201289	3.363314	4.372308	2.2	2.2	6.572308
1	0.428705	0.392505	0.428705	1.261034	2.50702594	3.193664	4.151763	2.2	2.2	6.351763
1	0.435728	0.392505	0.435728	1.156069	2.298348637	2.927833	3.806182	2.2	2.2	6.006182
1.5	0.904747	0.883135	0.904747	1.328021	2.640201289	1.494806	1.943248	2	3	4.943248
1.5	0.919335	0.883135	0.919335	1.261034	2.50702594	1.419406	1.845228	2	3	4.845228
1.5	0.926359	0.883135	0.926359	1.156069	2.298348637	1.301259	1.691637	2	3	4.691637
2	1.59163	1.570018	1.59163	1.328021	2.640201289	0.840828	1.093077	1.6	3.2	4.293077
2	1.606218	1.570018	1.606218	1.261034	2.50702594	0.798416	1.037941	1.6	3.2	4.237941
2	1.613242	1.570018	1.613242	1.156069	2.298348637	0.731958	0.951546	1.6	3.2	4.151546
2.5	2.474765	2.453153	2.474765	1.328021	2.640201289	0.53813	0.699569	1.4	3.5	4.199569
2.5	2.489353	2.453153	2.489353	1.261034	2.50702594	0.510986	0.664282	1.4	3.5	4.164282
2.5	2.496377	2.453153	2.496377	1.156069	2.298348637	0.468453	0.608989	1.4	3.5	4.108989
3	3.554153	3.532541	3.554153	1.328021	2.640201289	0.373702	0.485812	1.2	3.6	4.085812
3	3.568741	3.532541	3.568741	1.261034	2.50702594	0.354852	0.461307	1.2	3.6	4.061307
3	3.575765	3.532541	3.575765	1.156069	2.298348637	0.325315	0.422909	1.2	3.6	4.022909
3.5	4.829792	4.80818	4.829792	1.328021	2.640201289	0.274556	0.356923	1.1	3.85	4.206923

3.5	4.84438	4.80818	4.84438	1.261034	2.50702594	0.260707	0.338919	1.1	3.85	4.188919
3.5	4.851404	4.80818	4.851404	1.156069	2.298348637	0.239007	0.310709	1.1	3.85	4.160709
4	6.301684	6.280072	6.301684	1.328021	2.640201289	0.210207	0.273269	1	4	4.273269
4	6.316272	6.280072	6.316272	1.261034	2.50702594	0.199604	0.259485	1	4	4.259485
4	6.323296	6.280072	6.323296	1.156069	2.298348637	0.18299	0.237886	1	4	4.237886

Table 3.28: Calculation of gasifier height for 700 kg/hr at $U_{f\,=}$ 0. 4466

Basis mass flow rate: 700 kg/hr										
U_f = 0.4466										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.091422	0.116762	0.882724	1.753524	8.93	11.61	3.5	1.75	13.36
0.5	0.19625	0.091422	0.121679	0.809249	1.607566	8.19	10.64	3.5	1.75	12.39
0.5	0.19625	0.091422	0.10655	0.929615	1.846672	9.40	12.23	3.5	1.75	13.98
1	0.785	0.365688	0.391028	0.882724	1.753524	2.23	2.90	2.2	2.2	5.10
1	0.785	0.365688	0.395945	0.809249	1.607566	2.04	2.66	2.2	2.2	4.86
1	0.785	0.365688	0.380817	0.929615	1.846672	2.35	3.05	2.2	2.2	5.25
1.5	1.76625	0.822799	0.848139	0.882724	1.753524	0.99	1.29	2	3	4.29
1.5	1.76625	0.822799	0.853055	0.809249	1.607566	0.91	1.18	2	3	4.18
1.5	1.76625	0.822799	0.837927	0.929615	1.846672	1.04	1.35	2	3	4.35
2	3.14	1.462753	1.488093	0.882724	1.753524	0.55	0.72	1.6	3.2	3.92
2	3.14	1.462753	1.49301	0.809249	1.607566	0.51	0.66	1.6	3.2	3.86
2	3.14	1.462753	1.477881	0.929615	1.846672	0.58	0.76	1.6	3.2	3.96
2.5	4.90625	2.285551	2.310892	0.882724	1.753524	0.35	0.46	1.4	3.5	3.96

2.5	4.90625	2.285551	2.315808	0.809249	1.607566	0.32	0.42	1.4	3.5	3.92
2.5	4.90625	2.285551	2.30068	0.929615	1.846672	0.37	0.48	1.4	3.5	3.98
3	7.065	3.291194	3.316534	0.882724	1.753524	0.24	0.32	1.2	3.6	3.92
3	7.065	3.291194	3.321451	0.809249	1.607566	0.22	0.29	1.2	3.6	3.89
3	7.065	3.291194	3.306323	0.929615	1.846672	0.26	0.33	1.2	3.6	3.93
3.5	9.61625	4.479681	4.505021	0.882724	1.753524	0.18	0.23	1.1	3.85	4.08
3.5	9.61625	4.479681	4.509938	0.809249	1.607566	0.16	0.21	1.1	3.85	4.06
3.5	9.61625	4.479681	4.494809	0.929615	1.846672	0.19	0.24	1.1	3.85	4.09
4	12.56	5.851012	5.876352	0.882724	1.753524	0.13	0.18	1	4	4.18
4	12.56	5.851012	5.881269	0.809249	1.607566	0.12	0.16	1	4	4.16
4	12.56	5.851012	5.86614	0.929615	1.846672	0.14	0.19	1	4	4.19

Table 3.29: Calculation of gasifier height for 700 kg/hr at U_f = 0.4658

Basis mass flow rate: 700 kg/hr										
U_f = 0.4658										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.098126	0.123466	0.882724	1.753524	8.935153	11.6157	3.5	1.75	13.3657
0.5	0.19625	0.098126	0.128383	0.809249	1.607566	8.191417	10.64884	3.5	1.75	12.39884
0.5	0.19625	0.098126	0.113255	0.929615	1.846672	9.409796	12.23273	3.5	1.75	13.98273
1	0.785	0.392505	0.417845	0.882724	1.753524	2.233788	2.903925	2.2	2.2	5.103925
1	0.785	0.392505	0.422761	0.809249	1.607566	2.047854	2.662211	2.2	2.2	4.862211
1	0.785	0.392505	0.407633	0.929615	1.846672	2.352449	3.058184	2.2	2.2	5.258184
1.5	1.76625	0.883135	0.908475	0.882724	1.753524	0.992795	1.290633	2	3	4.290633

1.5	1.76625	0.883135	0.913392	0.809249	1.607566	0.910157	1.183205	2	3	4.183205
1.5	1.76625	0.883135	0.898264	0.929615	1.846672	1.045533	1.359193	2	3	4.359193
2	3.14	1.570018	1.595358	0.882724	1.753524	0.558447	0.725981	1.6	3.2	3.925981
2	3.14	1.570018	1.600275	0.809249	1.607566	0.511964	0.665553	1.6	3.2	3.865553
2	3.14	1.570018	1.585146	0.929615	1.846672	0.588112	0.764546	1.6	3.2	3.964546
2.5	4.90625	2.453153	2.478493	0.882724	1.753524	0.357406	0.464628	1.4	3.5	3.964628
2.5	4.90625	2.453153	2.48341	0.809249	1.607566	0.327657	0.425954	1.4	3.5	3.925954
2.5	4.90625	2.453153	2.468282	0.929615	1.846672	0.376392	0.489309	1.4	3.5	3.989309
3	7.065	3.532541	3.557881	0.882724	1.753524	0.248199	0.322658	1.2	3.6	3.922658
3	7.065	3.532541	3.562797	0.809249	1.607566	0.227539	0.295801	1.2	3.6	3.895801
3	7.065	3.532541	3.547669	0.929615	1.846672	0.261383	0.339798	1.2	3.6	3.939798
3.5	9.61625	4.80818	4.83352	0.882724	1.753524	0.18235	0.237055	1.1	3.85	4.087055
3.5	9.61625	4.80818	4.838437	0.809249	1.607566	0.167172	0.217323	1.1	3.85	4.067323
3.5	9.61625	4.80818	4.823309	0.929615	1.846672	0.192037	0.249648	1.1	3.85	4.099648
4	12.56	6.280072	6.305412	0.882724	1.753524	0.139612	0.181495	1	4	4.181495
4	12.56	6.280072	6.310329	0.809249	1.607566	0.127991	0.166388	1	4	4.166388
4	12.56	6.280072	6.295201	0.929615	1.846672	0.147028	0.191136	1	4	4.191136

Table 3.30: Calculation of gasifier height for 700 kg/hr at $U_{f\,=}$ 0. 5

Basis mass flow rate: 700 kg/hr										
U_f = 0.5										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.098126	0.123466	0.882724	1.753524	8.935153	11.6157	3.5	1.75	13.3657
0.5	0.19625	0.098126	0.128383	0.809249	1.607566	8.191417	10.64884	3.5	1.75	12.39884

0.5	0.19625	0.098126	0.113255	0.929615	1.846672	9.409796	12.23273	3.5	1.75	13.98273
1	0.785	0.392505	0.417845	0.882724	1.753524	2.233788	2.903925	2.2	2.2	5.103925
1	0.785	0.392505	0.422761	0.809249	1.607566	2.047854	2.662211	2.2	2.2	4.862211
1	0.785	0.392505	0.407633	0.929615	1.846672	2.352449	3.058184	2.2	2.2	5.258184
1.5	1.76625	0.883135	0.908475	0.882724	1.753524	0.992795	1.290633	2	3	4.290633
1.5	1.76625	0.883135	0.913392	0.809249	1.607566	0.910157	1.183205	2	3	4.183205
1.5	1.76625	0.883135	0.898264	0.929615	1.846672	1.045533	1.359193	2	3	4.359193
2	3.14	1.570018	1.595358	0.882724	1.753524	0.558447	0.725981	1.6	3.2	3.925981
2	3.14	1.570018	1.600275	0.809249	1.607566	0.511964	0.665553	1.6	3.2	3.865553
2	3.14	1.570018	1.585146	0.929615	1.846672	0.588112	0.764546	1.6	3.2	3.964546
2.5	4.90625	2.453153	2.478493	0.882724	1.753524	0.357406	0.464628	1.4	3.5	3.964628
2.5	4.90625	2.453153	2.48341	0.809249	1.607566	0.327657	0.425954	1.4	3.5	3.925954
2.5	4.90625	2.453153	2.468282	0.929615	1.846672	0.376392	0.489309	1.4	3.5	3.989309
3	7.065	3.532541	3.557881	0.882724	1.753524	0.248199	0.322658	1.2	3.6	3.922658
3	7.065	3.532541	3.562797	0.809249	1.607566	0.227539	0.295801	1.2	3.6	3.895801
3	7.065	3.532541	3.547669	0.929615	1.846672	0.261383	0.339798	1.2	3.6	3.939798
3.5	9.61625	4.80818	4.83352	0.882724	1.753524	0.18235	0.237055	1.1	3.85	4.087055
3.5	9.61625	4.80818	4.838437	0.809249	1.607566	0.167172	0.217323	1.1	3.85	4.067323
3.5	9.61625	4.80818	4.823309	0.929615	1.846672	0.192037	0.249648	1.1	3.85	4.099648
4	12.56	6.280072	6.305412	0.882724	1.753524	0.139612	0.181495	1	4	4.181495
4	12.56	6.280072	6.310329	0.809249	1.607566	0.127991	0.166388	1	4	4.166388
4	12.56	6.280072	6.295201	0.929615	1.846672	0.147028	0.191136	1	4	4.191136

Table 3.31: Calculation of gasifier height for 360 kg/hr at $U_{f} =$ 0. 4466

Basis mass flow rate: 360 kg/hr										
U_f = 0.4466										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.087652	0.100684	0.453972	0.901812	4.595221	5.973788	3.5	1.75	7.723788
0.5	0.19625	0.087652	0.103213	0.416185	0.826748	4.212729	5.476548	3.5	1.75	7.226548
0.5	0.19625	0.087652	0.095432	0.478088	0.949717	4.839323	6.29112	3.5	1.75	8.04112
1	0.785	0.350608	0.36364	0.453972	0.901812	1.148805	1.493447	2.2	2.2	3.693447
1	0.785	0.350608	0.366169	0.416185	0.826748	1.053182	1.369137	2.2	2.2	3.569137
1	0.785	0.350608	0.358389	0.478088	0.949717	1.209831	1.57278	2.2	2.2	3.77278
1.5	1.76625	0.788868	0.8019	0.453972	0.901812	0.51058	0.663754	2	3	3.663754
1.5	1.76625	0.788868	0.804429	0.416185	0.826748	0.468081	0.608505	2	3	3.608505
1.5	1.76625	0.788868	0.796649	0.478088	0.949717	0.537703	0.699013	2	3	3.699013
2	3.14	1.402433	1.415465	0.453972	0.901812	0.287201	0.373362	1.6	3.2	3.573362
2	3.14	1.402433	1.417993	0.416185	0.826748	0.263296	0.342284	1.6	3.2	3.542284
2	3.14	1.402433	1.410213	0.478088	0.949717	0.302458	0.393195	1.6	3.2	3.593195
2.5	4.90625	2.191301	2.204333	0.453972	0.901812	0.183809	0.238952	1.4	3.5	3.738952
2.5	4.90625	2.191301	2.206862	0.416185	0.826748	0.168509	0.219062	1.4	3.5	3.719062
2.5	4.90625	2.191301	2.199082	0.478088	0.949717	0.193573	0.251645	1.4	3.5	3.751645
3	7.065	3.155474	3.168506	0.453972	0.901812	0.127645	0.165939	1.2	3.6	3.765939
3	7.065	3.155474	3.171034	0.416185	0.826748	0.11702	0.152126	1.2	3.6	3.752126
3	7.065	3.155474	3.163254	0.478088	0.949717	0.134426	0.174753	1.2	3.6	3.774753
3.5	9.61625	4.29495	4.307982	0.453972	0.901812	0.09378	0.121914	1.1	3.85	3.971914

3.5	9.61625	4.29495	4.310511	0.416185	0.826748	0.085974	0.111766	1.1	3.85	3.961766
3.5	9.61625	4.29495	4.302731	0.478088	0.949717	0.098762	0.12839	1.1	3.85	3.97839
4	12.56	5.609731	5.622763	0.453972	0.901812	0.0718	0.09334	1	4	4.09334
4	12.56	5.609731	5.625292	0.416185	0.826748	0.065824	0.085571	1	4	4.085571
4	12.56	5.609731	5.617511	0.478088	0.949717	0.075614	0.098299	1	4	4.098299

Table 3.32: Calculation of gasifier height for 360 kg/hr at $U_{f\,=}$ 0.4658

Basis mass flow rate: 360 kg/hr										
U_f = 0. 4658										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.091422	0.104454	0.453972	0.901812	4.595221	5.973788	3.5	1.75	7.723788
0.5	0.19625	0.091422	0.106983	0.416185	0.826748	4.212729	5.476548	3.5	1.75	7.226548
0.5	0.19625	0.091422	0.099202	0.478088	0.949717	4.839323	6.29112	3.5	1.75	8.04112
1	0.785	0.365688	0.37872	0.453972	0.901812	1.148805	1.493447	2.2	2.2	3.693447
1	0.785	0.365688	0.381249	0.416185	0.826748	1.053182	1.369137	2.2	2.2	3.569137
1	0.785	0.365688	0.373469	0.478088	0.949717	1.209831	1.57278	2.2	2.2	3.77278
1.5	1.76625	0.822799	0.835831	0.453972	0.901812	0.51058	0.663754	2	3	3.663754
1.5	1.76625	0.822799	0.838359	0.416185	0.826748	0.468081	0.608505	2	3	3.608505
1.5	1.76625	0.822799	0.830579	0.478088	0.949717	0.537703	0.699013	2	3	3.699013
2	3.14	1.462753	1.475785	0.453972	0.901812	0.287201	0.373362	1.6	3.2	3.573362
2	3.14	1.462753	1.478314	0.416185	0.826748	0.263296	0.342284	1.6	3.2	3.542284
2	3.14	1.462753	1.470533	0.478088	0.949717	0.302458	0.393195	1.6	3.2	3.593195
2.5	4.90625	2.285551	2.298584	0.453972	0.901812	0.183809	0.238952	1.4	3.5	3.738952
2.5	4.90625	2.285551	2.301112	0.416185	0.826748	0.168509	0.219062	1.4	3.5	3.719062

2.5	4.90625	2.285551	2.293332	0.478088	0.949717	0.193573	0.251645	1.4	3.5	3.751645
3	7.065	3.291194	3.304226	0.453972	0.901812	0.127645	0.165939	1.2	3.6	3.765939
3	7.065	3.291194	3.306755	0.416185	0.826748	0.11702	0.152126	1.2	3.6	3.752126
3	7.065	3.291194	3.298974	0.478088	0.949717	0.134426	0.174753	1.2	3.6	3.774753
3.5	9.61625	4.479681	4.492713	0.453972	0.901812	0.09378	0.121914	1.1	3.85	3.971914
3.5	9.61625	4.479681	4.495242	0.416185	0.826748	0.085974	0.111766	1.1	3.85	3.961766
3.5	9.61625	4.479681	4.487461	0.478088	0.949717	0.098762	0.12839	1.1	3.85	3.97839
4	12.56	5.851012	5.864044	0.453972	0.901812	0.0718	0.09334	1	4	4.09334
4	12.56	5.851012	5.866572	0.416185	0.826748	0.065824	0.085571	1	4	4.085571
4	12.56	5.851012	5.858792	0.478088	0.949717	0.075614	0.098299	1	4	4.098299

Table 3.33: Calculation of gasifier height for 360 kg/hr at $U_{f\,=}$ 0.5

Basis mass flow rate: 360 kg/hr										
U_f = 0. 5										
dt	**Cross sectional area**	**Qex**	**Qtotal**	**Qcoal**	**Qcoal @ mf**	**Hmf**	**H**	**TDH/dt**	**TDH**	**Ht**
0.5	0.19625	0.098126	0.111158	0.453972	0.901812	4.595221	5.973788	3.5	1.75	7.723788
0.5	0.19625	0.098126	0.113687	0.416185	0.826748	4.212729	5.476548	3.5	1.75	7.226548
0.5	0.19625	0.098126	0.105906	0.478088	0.949717	4.839323	6.29112	3.5	1.75	8.04112
1	0.785	0.392505	0.405537	0.453972	0.901812	1.148805	1.493447	2.2	2.2	3.693447
1	0.785	0.392505	0.408065	0.416185	0.826748	1.053182	1.369137	2.2	2.2	3.569137
1	0.785	0.392505	0.400285	0.478088	0.949717	1.209831	1.57278	2.2	2.2	3.77278
1.5	1.76625	0.883135	0.896167	0.453972	0.901812	0.51058	0.663754	2	3	3.663754
1.5	1.76625	0.883135	0.898696	0.416185	0.826748	0.468081	0.608505	2	3	3.608505

1.5	1.76625	0.883135	0.890915	0.478088	0.949717	0.537703	0.699013	2	3	3.699013
2	3.14	1.570018	1.58305	0.453972	0.901812	0.287201	0.373362	1.6	3.2	3.573362
2	3.14	1.570018	1.585579	0.416185	0.826748	0.263296	0.342284	1.6	3.2	3.542284
2	3.14	1.570018	1.577798	0.478088	0.949717	0.302458	0.393195	1.6	3.2	3.593195
2.5	4.90625	2.453153	2.466185	0.453972	0.901812	0.183809	0.238952	1.4	3.5	3.738952
2.5	4.90625	2.453153	2.468714	0.416185	0.826748	0.168509	0.219062	1.4	3.5	3.719062
2.5	4.90625	2.453153	2.460934	0.478088	0.949717	0.193573	0.251645	1.4	3.5	3.751645
3	7.065	3.532541	3.545573	0.453972	0.901812	0.127645	0.165939	1.2	3.6	3.765939
3	7.065	3.532541	3.548101	0.416185	0.826748	0.11702	0.152126	1.2	3.6	3.752126
3	7.065	3.532541	3.540321	0.478088	0.949717	0.134426	0.174753	1.2	3.6	3.774753
3.5	9.61625	4.80818	4.821212	0.453972	0.901812	0.09378	0.121914	1.1	3.85	3.971914
3.5	9.61625	4.80818	4.823741	0.416185	0.826748	0.085974	0.111766	1.1	3.85	3.961766
3.5	9.61625	4.80818	4.815961	0.478088	0.949717	0.098762	0.12839	1.1	3.85	3.97839
4	12.56	6.280072	6.293104	0.453972	0.901812	0.0718	0.09334	1	4	4.09334
4	12.56	6.280072	6.295633	0.416185	0.826748	0.065824	0.085571	1	4	4.085571
4	12.56	6.280072	6.287853	0.478088	0.949717	0.075614	0.098299	1	4	4.098299

The tabulated results are graphically represented for each of three coal samples on representative basis to analyze the effect of changing diameter on the height of reactor at minimum fluidization velocity, H_{mf} (figures 3.7, 3.8 and 3.9), transport disengaging height, TDH (figures 3.10, 3.11 and 3.12), height of the Fluidized Bed Reactor, H_t (figures 3.13, 3.14, and 3.15).

The plots below show that, with enhancement in quality of coal, required height of fluidized bed also reduces, though, the difference is marginal. For larger operations requiring large diameter beds, the effect of coal quality becomes an unimportant parameter. Hence, the model developed and used in the present study becomes robust for any type of coal for medium to high capacity plants.

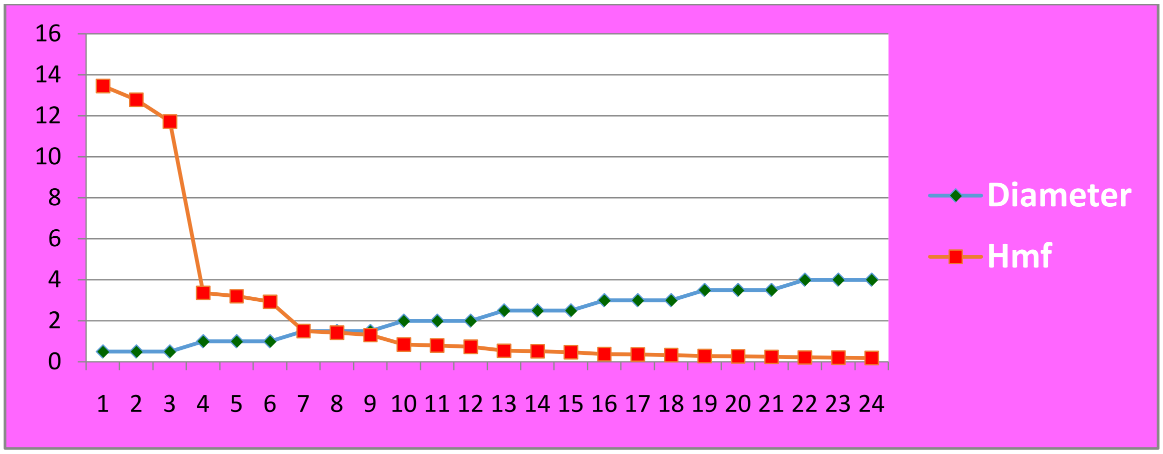


Fig. 3.7: Effect of diameter on H_{mf} for 1000 kg/hr at $U_{f\,=}$ 0.4466 for Lignite

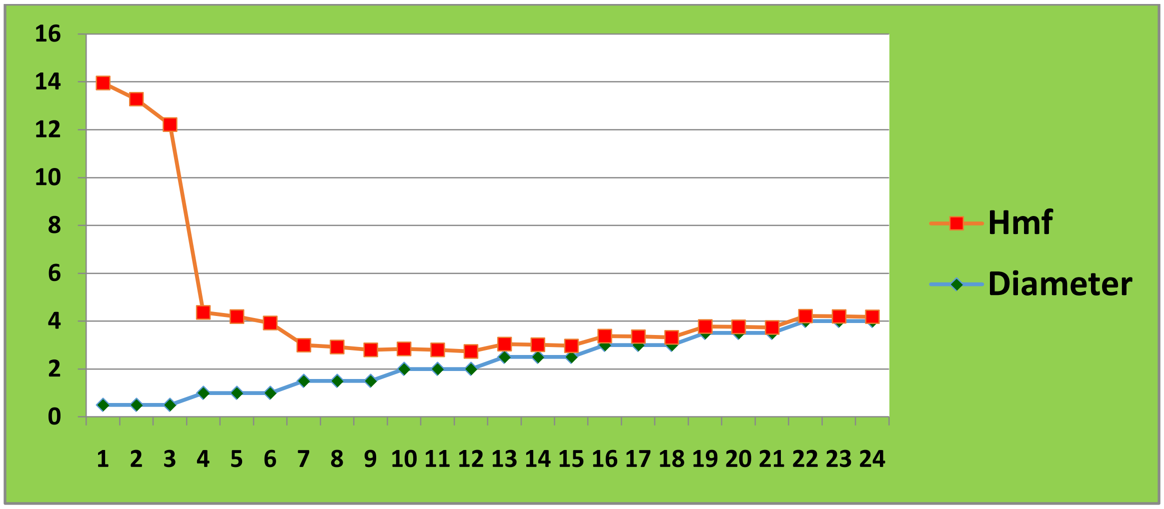


Fig. 3.8: Effect of diameter on H_{mf} for 1000 kg/hr at $U_{f\,=}$ 0.4685 for Bituminous

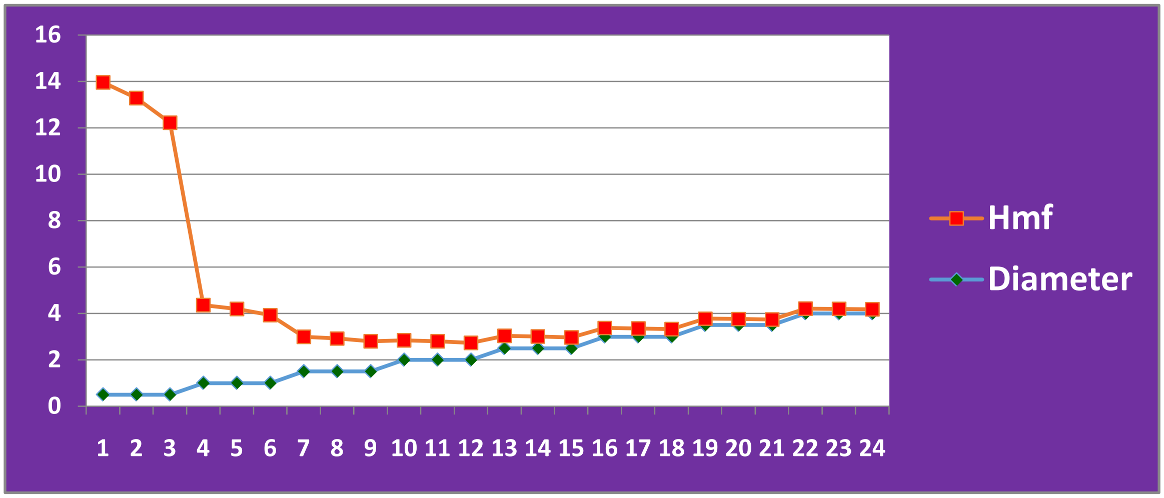


Fig. 3.9: Effect of diameter on H_{mf} for 360 kg/hr at $U_{f\,=}$ 0.5 for Anthracite coal

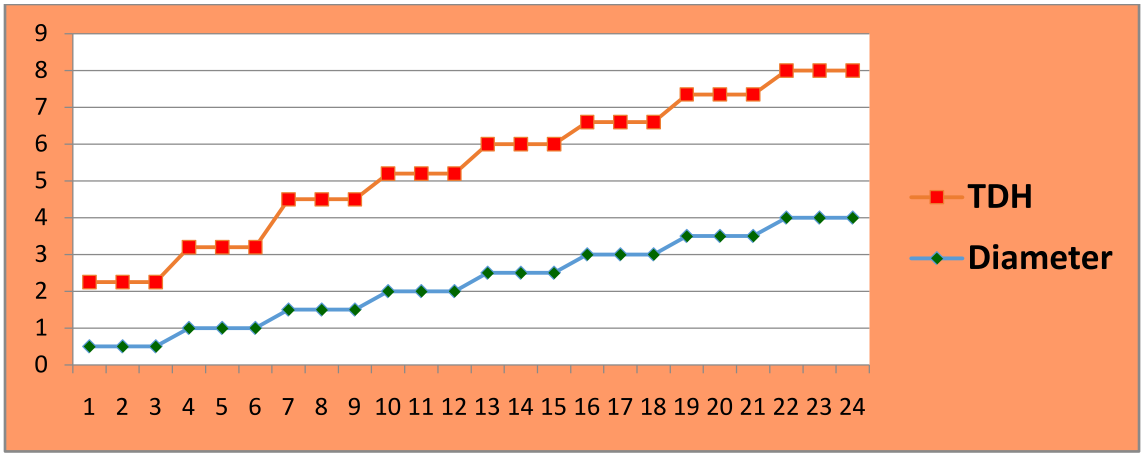


Fig. 3.10: Effect of diameter on TDH for 750 kg/hr at $U_{f} =$ 0.4466 for Lignite

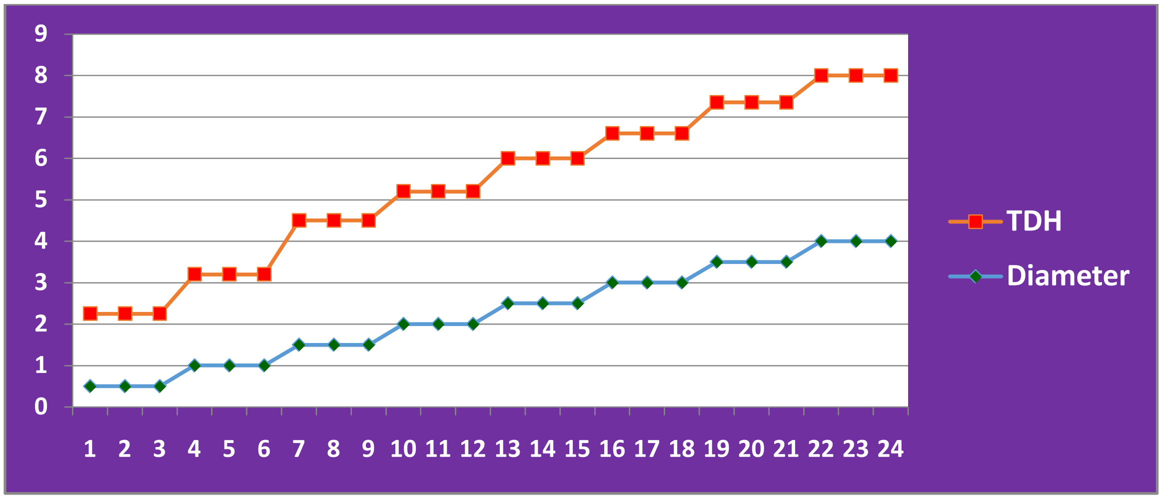


Fig. 3.11: Effect of diameter on TDH for 750 kg/hr at $U_{f} =$ 0.4685 for Bituminous

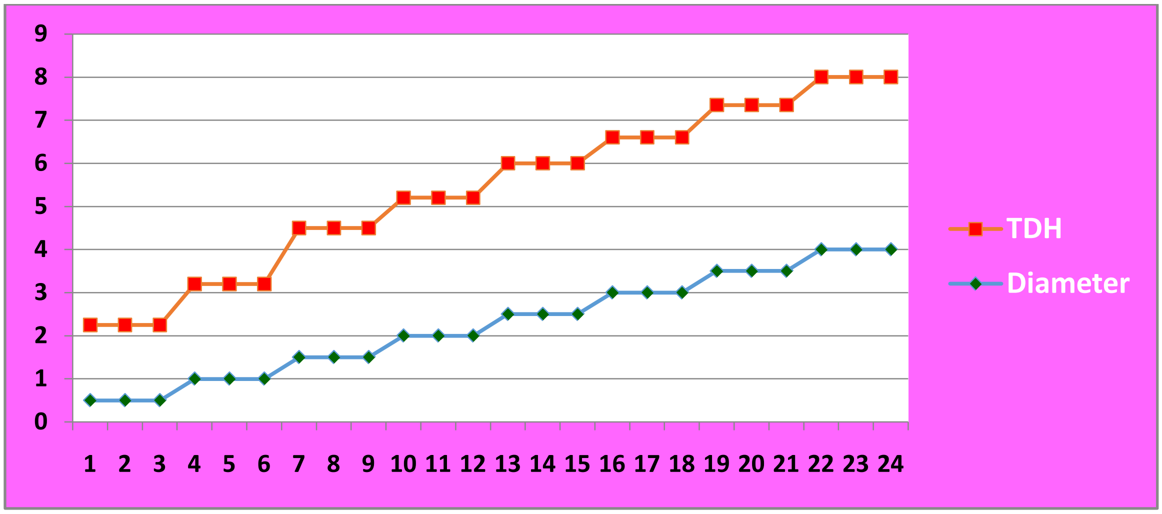


Fig. 3.12: Effect of diameter on TDH for 750 kg/hr at $U_{f} =$ 0.5 for Anthracite coal

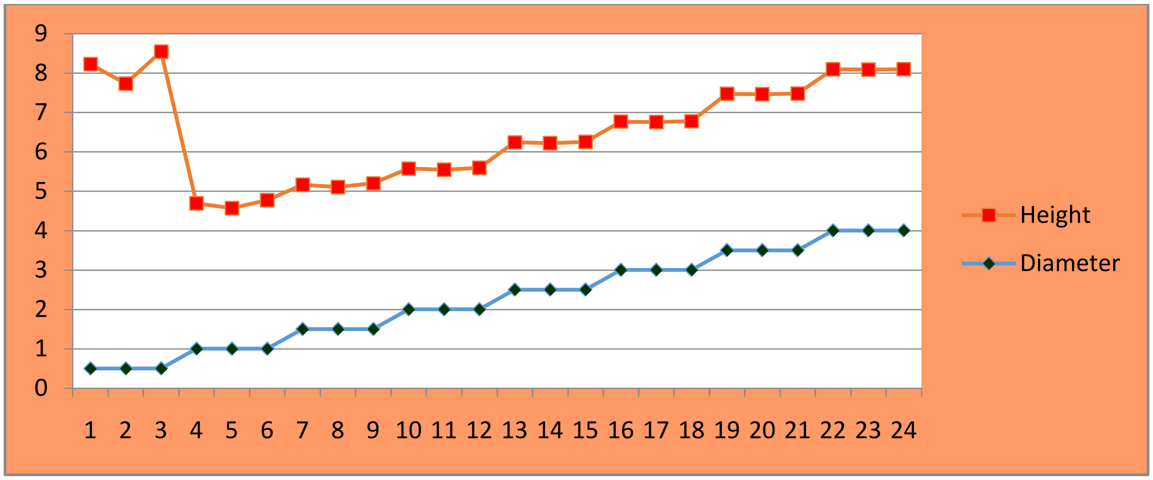


Fig. 3.13: Effect of diameter on gasifier height for 360 kg/hr at $U_{f} =$ 0.4466 for Lignite

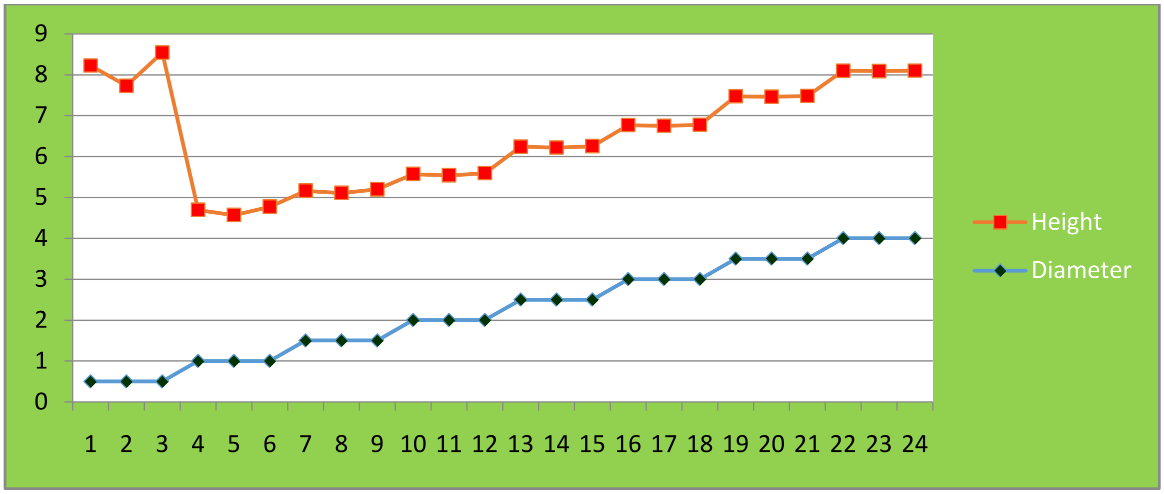


Fig. 3.14: Effect of diameter on gasifier height for 360 kg/hr at $U_{f} =$ 0.4685 for Bituminous coal

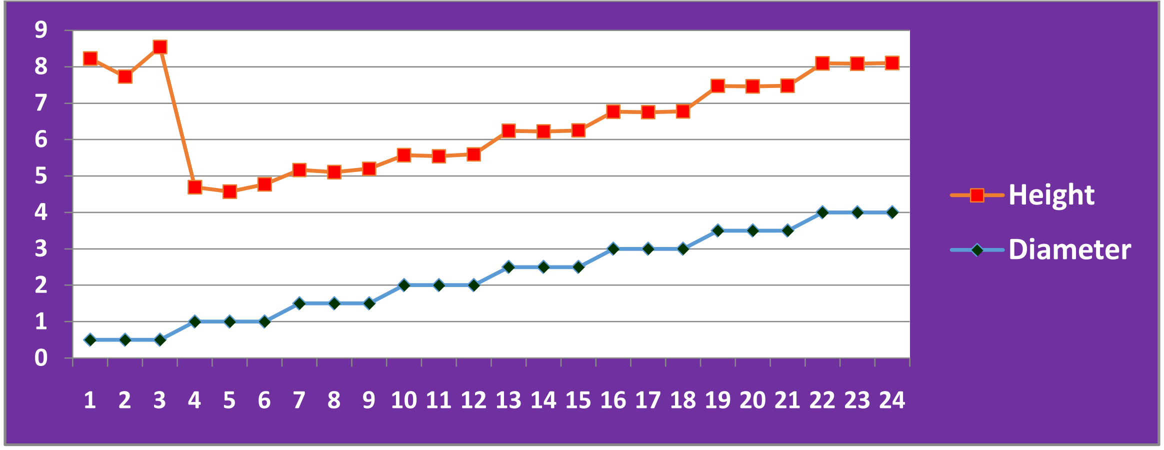


Fig. 3.15: Effect of diameter on gasifier height for 360 kg/hr at $U_{f} =$ 0.5 for Anthracite $U_{f} =$ 0.5 for Anthracite coal

From the present study, the coal density emerges as a prominent parameter affecting required height of fluidized bed. The effect is shown in figure 3.16. This is also in accordance with earlier studies performed on fluidized bed reactors for gasification [9].

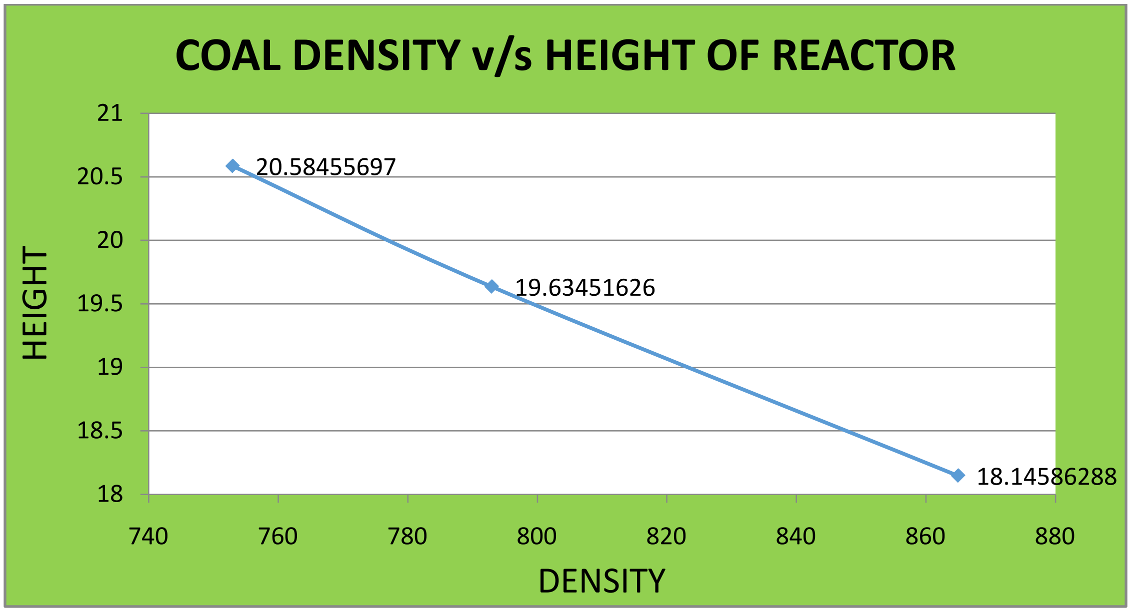


Fig. 3.16: Effect of coal density on gasifier height

3.7 Bubble Dynamics in Fluidized Bed:

In order to develop a first principle model which can be useful for control purposes, a number of simplifications and assumptions will be needed. However, it must be noticed that these assumptions are quite common in fluidization theory and they do not represent a serious deficiency in the final model [2, 9, 10, 15].

3.7.1 Behaviour in the vicinity of a single bubble: In the vicinity of any of the many rising bubbles in a bubbling fluidized bed let us assume that the gas flow is given by the Davidson model with its spherical bubble surrounded with a spherical cloud. The velocity of rise of a single bubble of diameter *dB,* hence the velocity relative to solids far from the bubble is

$$U_{br} = 0.711(gd_b)^{1/2}$$

Where, g is acceleration due to gravity

3.7.2 Bubble size: The importance of this parameter is critical for the mass and heat transfer coefficients. Therefore, it is very convenient to have an accurate estimation as well as information about reactor internals. To estimate the bubble diameter *dB* is chosen:

$$d_{BO} = 0.00376(U_o - U_{mf})^{1/2}$$

$$d_{BM} = 0.652\left(A\left(U_o - U_{mf}\right)\right)^{\frac{2}{5}}$$

Where d_{BO} is the initial bubble diameter at the surface of the perforated plate and d_{BM} is the bubble diameter if there were a single train of bubbles. Then

$$d_B = d_{BM} - (d_{BM} - d_{BO})\ e^{(-0.3z^*/D)}$$

Where *z'* is the position (height) in the bed, Umf is the minimum fluidization velocity and *Uo* is the inlet gas velocity. All *d's* must be in em and all *U's* in cm/s, because they are experimental correlations. However, this model requires four conditions:

$30 < D < 130$ cm
$0.5 <$ Umf < 20 cm/s
$0.006 < dp < 0.045$ cm
$Uo -$ Umf < 48 cm/s

Here, *dp* is a mean diameter of the particles. It must be carefully checked that the design characteristics of the reactor meet these requirements; otherwise this model could not be valid.

3.7.3 Bubble velocity: Let us relate the velocity of rise of a crowd of bubbles to the velocity of rise of a single bubble by

$$U_b = U_o - U_{mf} + U_{br} = U_o - U_{mf} + 0.711(gd_b)^{\frac{1}{2}}$$

Where

$$U_{br} = 0.711(gd_b)^{1/2}$$

3.7.4 Relative fraction of bubble phase to total volume in bed. With the assumptions presented above

$$\delta^* \approx \frac{U_o - U_{mf}}{U_b}$$

3.7.5 Velocity of emulsion gas. under the assumption that conditions in the emulsion phase at any flow rate are the same as at minimum fluidizing conditions, the following expression for the velocity of emulsion gas *Ue* is derived

$$U_e = \frac{U_{mf}}{\varepsilon_{mf}\,(1-\delta^*)}$$

3.7.6 Mass transfer coefficient bubble phase - emulsion. For this coefficient the Kunii-Levenspiel model [4]

$$K_{bc} = 4.5\,\frac{U_{mf}}{d_B} + 5.85\left(\frac{D^{\frac{1}{2}}g^{\frac{1}{4}}}{{d_B}^{3}}\right)$$

$$K_{ce} \approx 6.78\left(\frac{\varepsilon_{mf}\,D_e\,U_b}{{d_B}^{3}}\right)^{\frac{1}{2}}$$

where *Kbe* is the mass transfer coefficient bubble-cloud per unit bubble volume, *Kce* is the mass transfer coefficient cloud-emulsion per unit bubble volume and D, De are the diffusion and effective diffusion coefficients of the gas in emulsion. Then the mass transfer coefficient bubble-emulsion per unit bubble volume *Kbe* is determined from:

$$\frac{1}{K_{be}} \approx \frac{1}{K_{bc}} + \frac{1}{K_{ce}} \qquad \text{where } D \approx De$$

3.7.7 Heat transfer coefficient bubble phase – emulsion [30]:

The model proposed is:

$$H_{be} = 4.5\,\frac{U_{mf}\,.\,\rho_g\,.\,C_{\rho g}}{d_B} + 5.85\left(\frac{\left(k_g\,.\,\rho_g\,.\,C_{\rho g}\right)^{\frac{1}{2}}g^{\frac{1}{4}}}{{d_B}^{\frac{5}{4}}}\right)$$

$$H_{ce} = 6.78\left(k_g\,.\,\rho_g\,.\,C_{\rho g}\right)^{\frac{1}{2}}\left(\varepsilon_{mf}\,.\,\frac{U_b}{{d_B}^{3}}\right)^{\frac{1}{2}}$$

where H_{be} is the heat transfer coefficient bubble-cloud per unit bubble volume, H_{ce} is the heat transfer coefficient cloud-emulsion per unit bubble volume and *kg* is the heat conductivity of gas. Then the heat transfer coefficient bubble-emulsion per unit bubble volume H_{be} is determined by

$$\frac{1}{H_{be}} \approx \frac{1}{H_{bc}} + \frac{1}{H_{ce}}$$

3.7.8 Assumptions made for calculations

For calculating the bubble dynamics taking Cp_g (specific heat of gas, J/kg K)

$$Cp_g = 3.37 \text{J/(Kg K) (for steam and air)}$$

Thermal conductivity of gas as K_g (heat conductivity of gas J/(m s K))

$$K_g = 0.04 \text{ (J/ m s K) (for steam and air)}$$

And diffusivity of steam is

$$D \approx De = 0.000028 \text{ m}^2\text{/s}$$

Z* i.e. position (height) of bubble in the bed is calculated by taking 1/4th of the fluidized height H as bubble starts forming immediate after distributor plate.

$$Z^* = H/4$$

Table 3.34: Results for bubble dynamics calculations

Basis = 1000 kg/hr ε_{mf} = 0.503								
Z*	**A**	**U_o-U_{mf}**	**d_{BO}**	**d_{BM}**	**d_B**	**U_{br}**	**δ***	**U_e**
4.372	0.19625	0.35173	0.00047	0.2238	0.20759	1.01463	0.25742	0.2631
4.372	0.19625	0.3465	0.00045	0.22246	0.20635	1.0116	0.25514	0.27624
4.372	0.19625	0.3371	0.00043	0.22003	0.20409	1.00605	0.25098	0.29965
1.093	0.785	0.35173	0.00047	0.38965	0.10927	0.73615	0.32332	0.28873
1.093	0.785	0.3465	0.00045	0.38733	0.10861	0.73392	0.32071	0.3029
1.093	0.785	0.3371	0.00043	0.38309	0.10741	0.72985	0.31595	0.32812
0.485	1.76625	0.35173	0.00047	0.53895	0.05032	0.49957	0.41317	0.33293
0.485	1.76625	0.3465	0.00045	0.53574	0.05001	0.49802	0.41029	0.34892
0.485	1.76625	0.3371	0.00043	0.52988	0.04945	0.49521	0.40502	0.37724
0.273	3.14	0.35173	0.00047	0.67842	0.02769	0.37059	0.48694	0.38081
0.273	3.14	0.3465	0.00045	0.67438	0.02752	0.36941	0.484	0.39876
0.273	3.14	0.3371	0.00043	0.667	0.0272	0.36726	0.47859	0.43046
0.174	4.90625	0.35173	0.00047	0.81102	0.0173	0.2929	0.54563	0.42999
0.174	4.90625	0.3465	0.00045	0.80618	0.01719	0.29193	0.54274	0.44998
0.174	4.90625	0.3371	0.00043	0.79736	0.01698	0.29017	0.53741	0.4852
0.121	7.065	0.35173	0.00047	0.93837	0.01179	0.24178	0.59263	0.4796
0.121	7.065	0.3465	0.00045	0.93277	0.01171	0.24094	0.58985	0.50166

0.121	7.065	0.3371	0.00043	0.92257	0.01156	0.23942	0.58471	0.54046
0.089	9.61625	0.35173	0.00047	1.06153	0.00855	0.20591	0.63075	0.52911
0.089	9.61625	0.3465	0.00045	1.0552	0.00849	0.20516	0.6281	0.55327
0.089	9.61625	0.3371	0.00043	1.04365	0.00838	0.20381	0.62322	0.59569
0.068	12.56	0.35173	0.00047	1.1812	0.0065	0.17953	0.66206	0.57814
0.068	12.56	0.3465	0.00045	1.17416	0.00645	0.17885	0.65957	0.6044
0.068	12.56	0.3371	0.00043	1.16131	0.00636	0.1776	0.65495	0.65047

Table 3.35: Heat and mass transfer coefficients for 1000 kg/hr basis

Hbc	Hce	Hbe	Kbc	Kce	Kbe
5.736775	11.54526	3.832451	2.522661	0.315576	0.280488
4.601855	11.61417	3.29592	2.652288	0.31746	0.283524
4.855254	11.74236	3.43496	2.890011	0.320964	0.288881
9.291321	26.97411	6.910854	4.922076	0.737306	0.64125
9.560267	27.12693	7.06897	5.169676	0.741483	0.648473
10.05441	27.4111	7.356166	5.62384	0.749251	0.661165
22.71712	76.35003	17.50785	11.09428	2.086939	1.756521
23.32382	76.75456	17.88807	11.63655	2.097996	1.777521
24.43913	77.50609	18.58039	12.63154	2.118539	1.814255
45.50371	172.2833	35.99631	20.8358	4.709163	3.841038
46.64891	173.1637	36.74902	21.83067	4.73323	3.88985
48.75529	174.7967	38.12207	23.65696	4.777865	3.975047
78.92682	329.6552	63.68033	34.32758	9.01074	7.137261
80.83155	331.3363	64.97942	35.9372	9.056693	7.233697
84.33689	334.4471	67.35269	38.89364	9.141723	7.40194
123.9272	562.3697	101.5492	51.67305	15.37172	11.84736
126.8343	565.3193	103.5925	54.0633	15.45234	12.01751
132.1875	570.7632	107.3301	58.45645	15.60115	12.31457
181.0629	882.4609	150.2373	72.87369	24.12104	18.12252
185.2371	887.3381	153.2461	76.21226	24.25435	18.39894

192.928	896.3171	158.7564	82.35313	24.49978	18.88235
250.5136	1299.469	210.0247	97.83229	35.51947	26.05853
256.2405	1307.172	214.2432	102.2866	35.73003	26.48017
266.7989	1321.323	221.9776	110.487	36.11683	27.21921

Table 3.36: Results for bubble dynamics calculations

Basis = 700 kg/hr ε_{mf} = 0.503									
Z*	A	Uo-Umf	dBO	dBM	dB	Ub	Ubr	δ*	Ue
2.9039	0.09827	0.35173	0.00047	0.1713	0.17114	1.27298	0.92125	0.2763	0.26997
2.6622	0.1035	0.3465	0.00045	0.17002	0.16974	2.31785	1.97135	0.14949	0.24192
3.0582	0.1129	0.3371	0.00043	0.1677	0.16759	2.25892	1.92182	0.14923	0.26382
0.726	0.09827	0.35173	0.00047	0.3426	0.19943	3.07309	2.72136	0.11445	0.22063
0.6656	0.1035	0.3465	0.00045	0.34004	0.18725	2.74566	2.39916	0.1262	0.23548
0.7645	0.1129	0.3371	0.00043	0.3354	0.20157	3.11712	2.78002	0.10815	0.25166
0.3227	0.09827	0.35173	0.00047	0.5139	0.11727	1.29274	0.94102	0.27208	0.2684
0.2958	0.1035	0.3465	0.00045	0.51007	0.10784	1.14224	0.79574	0.30335	0.29536
0.3398	0.1129	0.3371	0.00043	0.5031	0.12008	1.32364	0.98654	0.25468	0.30114
0.1815	0.09827	0.35173	0.00047	0.6852	0.07111	0.69776	0.34603	0.50408	0.39397
0.1664	0.1035	0.3465	0.00045	0.68009	0.06502	0.63581	0.28931	0.54498	0.45219
0.1911	0.1129	0.3371	0.00043	0.6708	0.07306	0.70236	0.36526	0.47996	0.43159
0.1162	0.09827	0.35173	0.00047	0.85649	0.04689	0.50215	0.15042	0.70044	0.65221
0.1065	0.1035	0.3465	0.00045	0.85011	0.04279	0.47179	0.12528	0.73445	0.77484
0.1223	0.1129	0.3371	0.00043	0.8385	0.04822	0.4962	0.1591	0.67937	0.70002
0.0807	0.09827	0.35173	0.00047	1.02779	0.03308	0.42662	0.07489	0.82445	1.11295
0.074	0.1035	0.3465	0.00045	1.02013	0.03017	0.40879	0.06229	0.84763	1.35034
0.0849	0.1129	0.3371	0.00043	1.0062	0.03403	0.41634	0.07923	0.80969	1.17936
0.0593	0.09827	0.35173	0.00047	1.19909	0.02457	0.39305	0.04132	0.89487	1.85843
0.0543	0.1035	0.3465	0.00045	1.19016	0.02241	0.38086	0.03436	0.90979	2.28096
0.0624	0.1129	0.3371	0.00043	1.1739	0.02527	0.3808	0.0437	0.88525	1.95596
0.0454	0.09827	0.35173	0.00047	1.37039	0.01899	0.37639	0.02467	0.93447	2.98138
0.0416	0.1035	0.3465	0.00045	1.36018	0.01731	0.36702	0.02051	0.94411	3.68154
0.0478	0.1129	0.3371	0.00043	1.3416	0.01952	0.36316	0.02606	0.92824	3.12766

Table 3.37: Heat and mass transfer coefficients for 700 kg/hr basis

Z*	A	Uo-Umf	dBO	dBM	dB	Ub	Ubr	δ*	Ue
2.9039	0.09827	0.35173	0.00047	0.1713	0.17114	1.27298	0.92125	0.2763	0.26997
2.6622	0.1035	0.3465	0.00045	0.17002	0.16974	2.31785	1.97135	0.14949	0.24192
3.0582	0.1129	0.3371	0.00043	0.1677	0.16759	2.25892	1.92182	0.14923	0.26382
0.726	0.09827	0.35173	0.00047	0.3426	0.19943	3.07309	2.72136	0.11445	0.22063
0.6656	0.1035	0.3465	0.00045	0.34004	0.18725	2.74566	2.39916	0.1262	0.23548
0.7645	0.1129	0.3371	0.00043	0.3354	0.20157	3.11712	2.78002	0.10815	0.25166
0.3227	0.09827	0.35173	0.00047	0.5139	0.11727	1.29274	0.94102	0.27208	0.2684
0.2958	0.1035	0.3465	0.00045	0.51007	0.10784	1.14224	0.79574	0.30335	0.29536
0.3398	0.1129	0.3371	0.00043	0.5031	0.12008	1.32364	0.98654	0.25468	0.30114
0.1815	0.09827	0.35173	0.00047	0.6852	0.07111	0.69776	0.34603	0.50408	0.39397
0.1664	0.1035	0.3465	0.00045	0.68009	0.06502	0.63581	0.28931	0.54498	0.45219
0.1911	0.1129	0.3371	0.00043	0.6708	0.07306	0.70236	0.36526	0.47996	0.43159
0.1162	0.09827	0.35173	0.00047	0.85649	0.04689	0.50215	0.15042	0.70044	0.65221
0.1065	0.1035	0.3465	0.00045	0.85011	0.04279	0.47179	0.12528	0.73445	0.77484
0.1223	0.1129	0.3371	0.00043	0.8385	0.04822	0.4962	0.1591	0.67937	0.70002
0.0807	0.09827	0.35173	0.00047	1.02779	0.03308	0.42662	0.07489	0.82445	1.11295
0.074	0.1035	0.3465	0.00045	1.02013	0.03017	0.40879	0.06229	0.84763	1.35034
0.0849	0.1129	0.3371	0.00043	1.0062	0.03403	0.41634	0.07923	0.80969	1.17936
0.0593	0.09827	0.35173	0.00047	1.19909	0.02457	0.39305	0.04132	0.89487	1.85843
0.0543	0.1035	0.3465	0.00045	1.19016	0.02241	0.38086	0.03436	0.90979	2.28096
0.0624	0.1129	0.3371	0.00043	1.1739	0.02527	0.3808	0.0437	0.88525	1.95596
0.0454	0.09827	0.35173	0.00047	1.37039	0.01899	0.37639	0.02467	0.93447	2.98138
0.0416	0.1035	0.3465	0.00045	1.36018	0.01731	0.36702	0.02051	0.94411	3.68154
0.0478	0.1129	0.3371	0.00043	1.3416	0.01952	0.36316	0.02606	0.92824	3.12766

Table 3.38: Results for bubble dynamics calculations

Basis = 360 kg/hr ε_{mf} = 0.503									
Z*	**A**	**Uo-Umf**	**dBO**	**dBM**	**Db**	**Ub**	**Ubr**	**δ***	**Ue**
1.4934	0.19625	0.35173	0.00047	0.1713	0.16656	1.26056	0.90884	0.27902	0.27099
1.3691	0.19625	0.3465	0.00045	0.17002	0.16368	1.24745	0.90095	0.27777	0.28489
1.5728	0.19625	0.3371	0.00043	0.1677	0.16386	1.23856	0.90145	0.27217	0.30838
0.3734	0.785	0.35173	0.00047	0.3426	0.12402	1.13595	0.78423	0.30963	0.283
0.3423	0.785	0.3465	0.00045	0.34004	0.11484	1.10116	0.75466	0.31467	0.30023
0.3932	0.785	0.3371	0.00043	0.3354	0.12643	1.12891	0.79181	0.29861	0.32
0.1659	1.76625	0.35173	0.00047	0.5139	0.06429	0.91639	0.56466	0.38382	0.31708
0.1521	1.76625	0.3465	0.00045	0.51007	0.05885	0.88672	0.54021	0.39077	0.33774
0.1748	1.76625	0.3371	0.00043	0.5031	0.06601	0.90926	0.57215	0.37075	0.35669
0.0933	3.14	0.35173	0.00047	0.6852	0.03776	0.78445	0.43273	0.44837	0.35418
0.0856	3.14	0.3465	0.00045	0.68009	0.03447	0.75993	0.41342	0.45597	0.37821
0.0983	3.14	0.3371	0.00043	0.6708	0.03882	0.77588	0.43878	0.43448	0.39689
0.0597	4.90625	0.35173	0.00047	0.85649	0.02466	0.70145	0.34972	0.50143	0.39187
0.0548	4.90625	0.3465	0.00045	0.85011	0.0225	0.68051	0.33401	0.50918	0.41922
0.0629	4.90625	0.3371	0.00043	0.8385	0.02536	0.69171	0.35461	0.48735	0.43781
0.0415	7.065	0.35173	0.00047	1.02779	0.01737	0.64524	0.29351	0.54511	0.4295
0.038	7.065	0.3465	0.00045	1.02013	0.01585	0.62683	0.28033	0.55279	0.46009
0.0437	7.065	0.3371	0.00043	1.0062	0.01785	0.63464	0.29753	0.53118	0.47875
0.0305	9.61625	0.35173	0.00047	1.19909	0.01293	0.6049	0.25318	0.58146	0.4668
0.0279	9.61625	0.3465	0.00045	1.19016	0.01179	0.58835	0.24185	0.58894	0.50056
0.0321	9.61625	0.3371	0.00043	1.1739	0.01327	0.59364	0.25653	0.56786	0.51938
0.0233	12.56	0.35173	0.00047	1.37039	0.01002	0.57466	0.22294	0.61206	0.50362
0.0214	12.56	0.3465	0.00045	1.36018	0.00915	0.55952	0.21302	0.61929	0.54045
0.0246	12.56	0.3371	0.00043	1.3416	0.01028	0.56288	0.22577	0.59889	0.55957

Table 3.39: Heat and mass transfer coefficients for 360 kg/hr basis

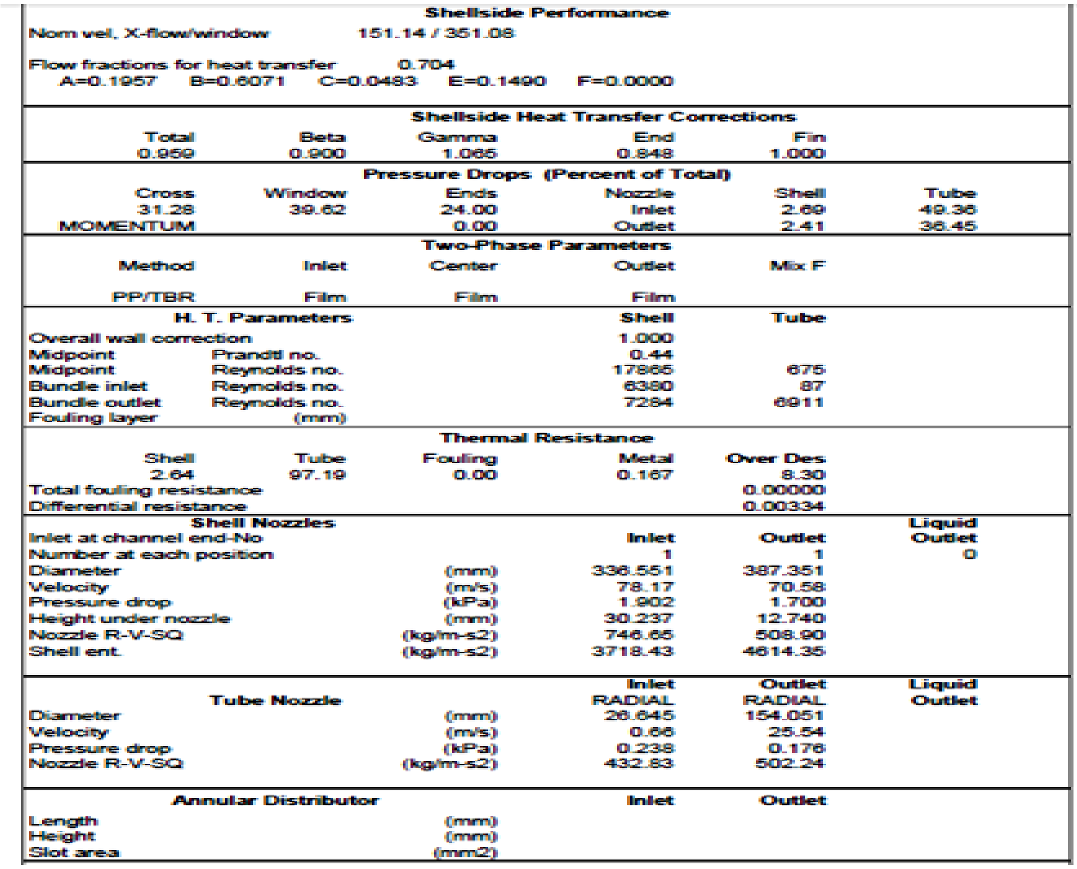
Hbc	Hce	Hbe	Kbc	Kce	Kbe
5.736775	15.43033	4.181976	3.171857	0.439113	0.385715
5.987469	15.75646	4.338743	3.373493	0.44938	0.396555
6.223459	15.6739	4.454687	3.627732	0.446151	0.397291
8.036799	22.79848	5.942116	4.313029	0.609839	0.534293
8.969827	25.18957	6.614464	4.877882	0.682013	0.598352
8.352718	22.08095	6.06026	4.747771	0.58676	0.52222
17.11068	54.85653	13.0425	8.576594	1.445204	1.236797
19.33081	61.62346	14.71487	9.811261	1.643846	1.407949
17.53802	52.5236	13.14785	9.339348	1.37358	1.197463
31.70846	112.7695	24.74943	15.01516	2.957818	2.471049
35.90446	127.2776	28.00451	17.21548	3.376734	2.823014
32.3005	107.5764	24.84164	16.2767	2.801678	2.390249
52.09999	202.013	41.41809	23.5568	5.293402	4.322175
59.00067	228.4032	46.88852	27.01376	6.047049	4.941002
52.88588	192.4257	41.48439	25.46916	5.008743	4.185605
78.53851	327.7401	63.35608	34.17445	8.591738	6.865656
88.88926	370.7906	71.70056	39.1701	9.81156	7.846198
79.5497	312.0409	63.38958	36.8861	8.12943	6.661323
111.1781	494.4457	90.76843	46.82982	12.97632	10.16081
125.721	559.4279	102.6519	53.63296	14.80693	11.60346
112.4611	470.8377	90.7784	50.48981	12.28494	9.880793
150.0695	705.8625	123.758	61.46539	18.55104	14.25016
169.526	798.3879	139.8342	70.32765	21.14613	16.25775
151.6954	672.5774	123.7781	66.22535	17.57982	13.8921

3.8 SHELL AND TUBE HEAT EXCHANGER DESIGN USING HTRI®

Assuming the exiting producer gas at 800°C after giving some of its heat to the economizer is to be cooled further down to 600°C; which has a composition as follows:

Carbon monoxide	55.83 kmol
Hydrogen	85.21 kmol
Carbon dioxide	11.17 kmol

Water at 20°C is used to form a steam at the receiving end of heat exchanger. HTRI design datasheets are shown in figures 3.17 and 3.18.



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                                   Shellside Performance
Nom vel, X-flow/window          151.14 / 351.08

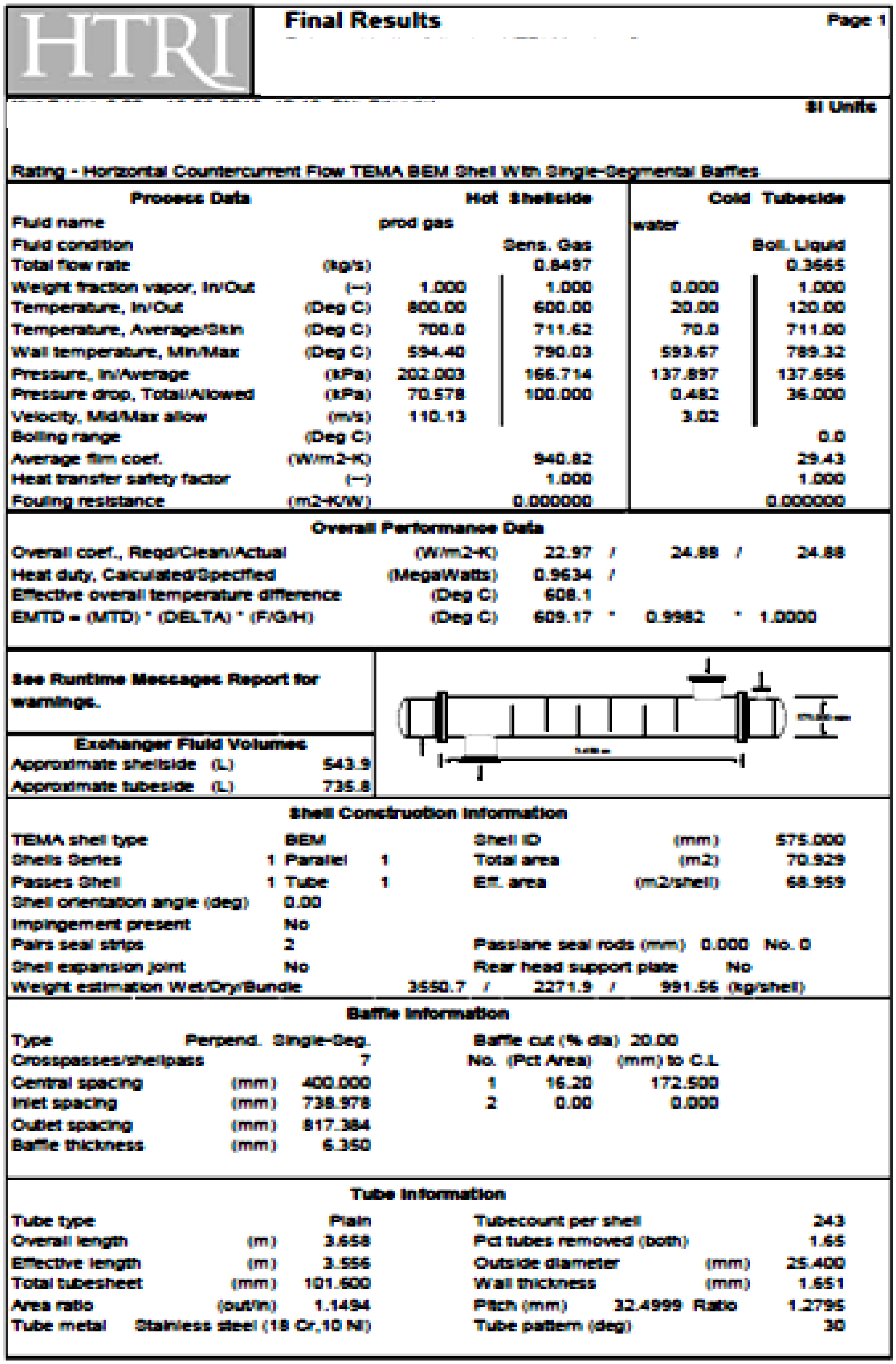
Flow fractions for heat transfer        0.704
    A=0.1957     B=0.6071     C=0.0483     E=0.1490     F=0.0000
                               Shellside Heat Transfer Corrections
             Total          Beta          Gamma          End          Fin
             0.959          0.900         1.065          0.848        1.000
                            Pressure Drops  (Percent of Total)
             Cross          Window         Ends          Nozzle        Shell          Tube
             31.28          39.62          24.00         Inlet         2.69           49.36
    MOMENTUM                               0.00          Outlet        2.41           36.45
                                   Two-Phase Parameters
            Method          Inlet          Center         Outlet        Mix F

            PP/TBR          Film           Film           Film
                 H. T. Parameters                         Shell         Tube
Overall wall correction                                   1.000
Midpoint             Prandtl no.                          0.44
Midpoint             Reynolds no.                         17865         675
Bundle inlet         Reynolds no.                         6380          87
Bundle outlet        Reynolds no.                         7284          6911
Fouling layer                  (mm)
                                   Thermal Resistance
             Shell          Tube           Fouling        Metal         Over Des
             2.64           97.19          0.00           0.167         8.30
Total fouling resistance                                                0.00000
Differential resistance                                                 0.00334
                 Shell Nozzles                                                         Liquid
Inlet at channel end-No                                   Inlet         Outlet         Outlet
Number at each position                                   1             1              0
Diameter                                   (mm)           336.551       387.351
Velocity                                   (m/s)          78.17         70.58
Pressure drop                              (kPa)          1.902         1.700
Height under nozzle                        (mm)           30.237        12.740
Nozzle R-V-SQ                              (kg/m-s2)      746.65        508.90
Shell ent.                                 (kg/m-s2)      3718.43       4614.35

                                                          Inlet         Outlet         Liquid
                  Tube Nozzle                             RADIAL        RADIAL         Outlet
Diameter                                   (mm)           26.645        154.051
Velocity                                   (m/s)          0.66          25.54
Pressure drop                              (kPa)          0.238         0.176
Nozzle R-V-SQ                              (kg/m-s2)      432.83        502.24

                 Annular Distributor                      Inlet         Outlet
Length                                     (mm)
Height                                     (mm)
Slot area                                  (mm2)
```

Fig. 3.17: Gasifier parameters obtained using HTRI



HTRI **Final Results** Page 1

SI Units

Rating - Horizontal Countercurrent Flow TEMA BEM Shell With Single-Segmental Baffles

Process Data		Hot Shellside		Cold Tubeside	
Fluid name		prod gas		water	
Fluid condition			Sens. Gas		Boil. Liquid
Total flow rate	(kg/s)		0.8497		0.3665
Weight fraction vapor, In/Out	(--)	1.000	1.000	0.000	1.000
Temperature, In/Out	(Deg C)	800.00	600.00	20.00	120.00
Temperature, Average/Skin	(Deg C)	700.0	711.62	70.0	711.00
Wall temperature, Min/Max	(Deg C)	594.40	790.03	593.67	789.32
Pressure, In/Average	(kPa)	202.003	166.714	137.897	137.656
Pressure drop, Total/Allowed	(kPa)	70.578	100.000	0.482	36.000
Velocity, Mid/Max allow	(m/s)	110.13		3.02	
Boiling range	(Deg C)				0.0
Average film coef.	(W/m2-K)		940.82		29.43
Heat transfer safety factor	(--)		1.000		1.000
Fouling resistance	(m2-K/W)		0.000000		0.000000

Overall Performance Data

Overall coef., Reqd/Clean/Actual	(W/m2-K)	22.97	/	24.88	/	24.88
Heat duty, Calculated/Specified	(MegaWatts)	0.9634	/			
Effective overall temperature difference	(Deg C)	608.1				
EMTD = (MTD) * (DELTA) * (F/G/H)	(Deg C)	609.17	*	0.9982	*	1.0000

See Runtime Messages Report for warnings.

Exchanger Fluid Volumes

Approximate shellside	(L)	543.9
Approximate tubeside	(L)	735.8

Shell Construction Information

TEMA shell type	BEM		Shell ID	(mm)	575.000
Shells Series	1 Parallel	1	Total area	(m2)	70.929
Passes Shell	1 Tube	1	Eff. area	(m2/shell)	68.959
Shell orientation angle (deg)	0.00				
Impingement present	No				
Pairs seal strips	2		Passlane seal rods (mm)	0.000	No. 0
Shell expansion joint	No		Rear head support plate	No	
Weight estimation Wet/Dry/Bundle	3550.7 /	2271.9 /	991.56 (kg/shell)		

Baffle Information

Type		Perpend. Single-Seg.	Baffle cut (% dia)	20.00	
Crosspasses/shellpass		7	No.	(Pct Area)	(mm) to C.L
Central spacing	(mm)	400.000	1	16.20	172.500
Inlet spacing	(mm)	738.978	2	0.00	0.000
Outlet spacing	(mm)	817.384			
Baffle thickness	(mm)	6.350			

Tube Information

Tube type		Plain	Tubecount per shell		243
Overall length	(m)	3.658	Pct tubes removed (both)		1.65
Effective length	(m)	3.556	Outside diameter	(mm)	25.400
Total tubesheet	(mm)	101.600	Wall thickness	(mm)	1.651
Area ratio	(out/in)	1.1494	Pitch (mm) 32.4999 Ratio		1.2795
Tube metal		Stainless steel (18 Cr,10 Ni)	Tube pattern (deg)		30

Fig. 3.18: Gasifier geometry obtained using HTRI

3.9 RESULTS AND DISCUSSIONS

- With equilibrium modeling of coal gasification reactions, H_2 to CO ratio stands at around 1.5 at 1500 K which can be enhanced as per the requirement with the help of optimization techniques [31].
- Heat and mass transfer parameters of the bed and gases in the column are as follows:

Table 3.40: Heat and mass transfer parameters of the bed and gases

Heat transfer coefficients		
Basis Kg/hr		
360	700	1000
Hbe		
4.181976	4.049193	3.832451
4.338743	4.479605	3.29592
4.454687	4.679598	3.43496
5.942116	3.725672	6.910854
6.614464	4.049175	7.06897
6.06026	3.876672	7.356166
13.0425	6.471792	17.50785
14.71487	7.183075	17.88807
13.14785	6.595364	18.58039
24.74943	11.11614	35.99631
28.00451	12.45341	36.74902
24.84164	11.20141	38.12207
41.41809	17.89224	63.68033
46.88852	20.1658	64.97942
41.48439	17.90849	67.35269
63.35608	27.0984	101.5492

Mass transfer coefficients		
Basis Kg/hr		
360	700	1000
Kbe		
0.385715	0.359495	0.280488
0.396555	0.474688	0.283524
0.397291	0.48313	0.288881
0.534293	0.421978	0.64125
0.598352	0.443279	0.648473
0.52222	0.425731	0.661165
1.236797	0.624236	1.756521
1.407949	0.671303	1.777521
1.197463	0.618831	1.814255
2.471049	0.981659	3.841038
2.823014	1.078143	3.88985
2.390249	0.959812	3.975047
4.322175	1.550983	7.137261
4.941002	1.731274	7.233697
4.185605	1.502006	7.40194
6.865656	2.388218	11.84736

This can be realized more satisfactorily in real life systems with rigorous modeling of heat transfer mechanisms.

- In this study, conditions are studied considering bubbling regime of fluidized bed systems and hence parameters like total bed height(Ht), total disengaging height (TDH) , bubbling rise velocities (*Ubr*), etc. are worked out.

Table 3.41: Bubble rise velocity

BASIS Kg/hr		
360	**700**	**1000**
Ubr		
0.908836	0.92125	1.014634
0.900951	1.971351	1.011601
0.901454	1.921819	1.006049
0.784226	2.721361	0.736146
0.754661	2.399156	0.73392
0.79181	2.780016	0.729847
0.56466	0.941017	0.499567
0.540214	0.795739	0.498025
0.572154	0.986536	0.495205
0.432727	0.346032	0.370587
0.413423	0.289311	0.369409
0.438777	0.365255	0.367258
0.349722	0.150424	0.292897
0.334007	0.125284	0.291931
0.354609	0.159095	0.290168
0.293513	0.074892	0.241776
0.280327	0.06229	0.240942
0.297532	0.079234	0.239424
0.253177	0.041321	0.20591
0.241847	0.034356	0.205163
0.256535	0.043697	0.203806
0.222935	0.024666	0.179534
0.213017	0.020512	0.178847
0.225773	0.026061	0.177599

Table 3.42: TDH and total column height

	Basis kg/hr		
	360	700	1000
TDH	Total column height, Ht		
1.75	7.723788	13.3657	19.23923
1.75	7.226548	12.39884	18.35705
1.75	8.04112	13.98273	16.97473
2.2	3.693447	5.103925	6.572308
2.2	3.569137	4.862211	6.351763
2.2	3.77278	5.258184	6.006182
3	3.663754	4.290633	4.943248
3	3.608505	4.183205	4.845228
3	3.699013	4.359193	4.691637
3.2	3.573362	3.925981	4.293077
3.2	3.542284	3.865553	4.237941
3.2	3.593195	3.964546	4.151546
3.5	3.738952	3.964628	4.199569
3.5	3.719062	3.925954	4.164282
3.5	3.751645	3.989309	4.108989
3.6	3.765939	3.922658	4.085812
3.6	3.752126	3.895801	4.061307
3.6	3.774753	3.939798	4.022909
3.85	3.971914	4.087055	4.206923
3.85	3.961766	4.067323	4.188919
3.85	3.97839	4.099648	4.160709
4	4.09334	4.181495	4.273269
4	4.085571	4.166388	4.259485
4	4.098299	4.191136	4.237886

.

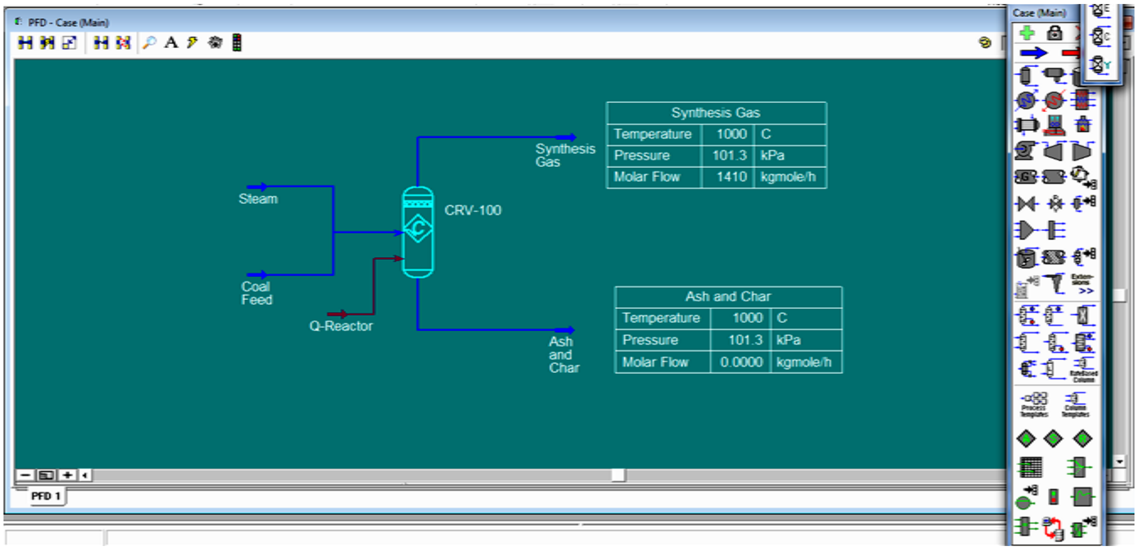
As with many efforts, the H_2 / CO ratio could not be enhanced than 1.5. Considering the same, it was thought to use Aspen HYSYS® simulation package to see whether the ratio can be enhanced further.

The simulation details are provided in section 3.10.

3.10 SIMULATION OF FLUIDIZED BED REACTOR

A coal gasification process model was developed and applied to study the generation of efficient, clean SYNTHESIS GAS (Syngas), as a feedstock for F-T synthesis and also for power generation. Identification of main units is basic steps for the process analysis. Thermodynamic databases, parametric models and steady state simulation software are fundamental tools, which are appropriately combined to gain the specific advantages**.**

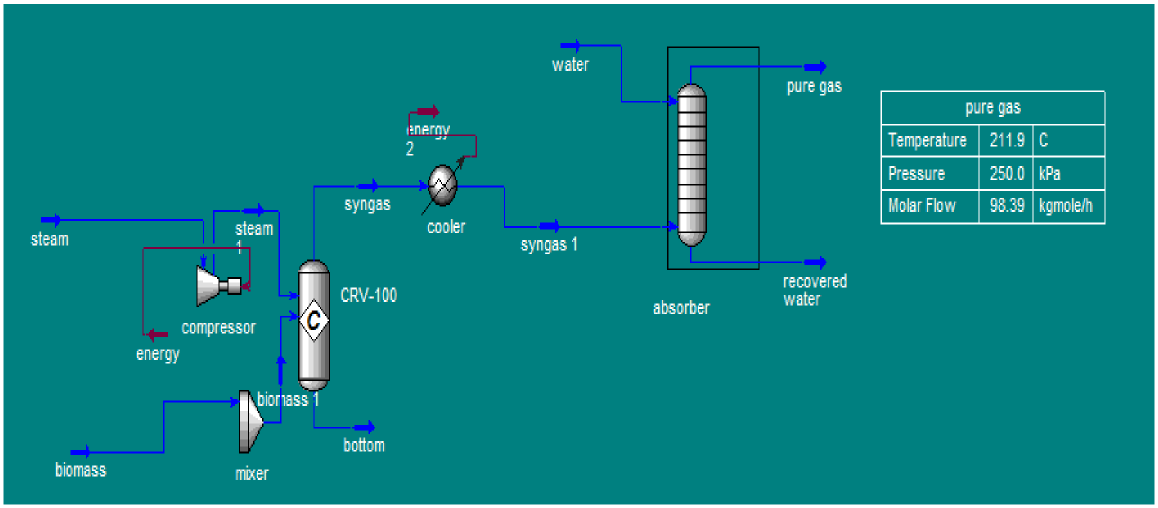
A simulation study using Aspen HYSYS® was performed considering coal samples. Using their proximate analysis and ultimate analysis, effects of various operating parameters on the process was studied and analyzed in order to enhance H_2 / CO ratio of the syngas. Simulation runs were carried out by varying different parameters like feed inlet pressure, flowrates, pressure drop across gas turbine, H_2 / CO ratio and thus results were generated. Aspen HYSYS® simulator provided a great help in analyzing the performance of unit operations. Figures 3.19 through 3.23 demonstrate the various steps involved in simulation. Steps for general simulation are already elaborated in chapter 2 while simulating complete power plant. Hence, specific steps are only indicated which are forming completely different base of simulation than referred earlier.



Synthesis Gas		
Temperature	1000	C
Pressure	101.3	kPa
Molar Flow	1410	kgmole/h

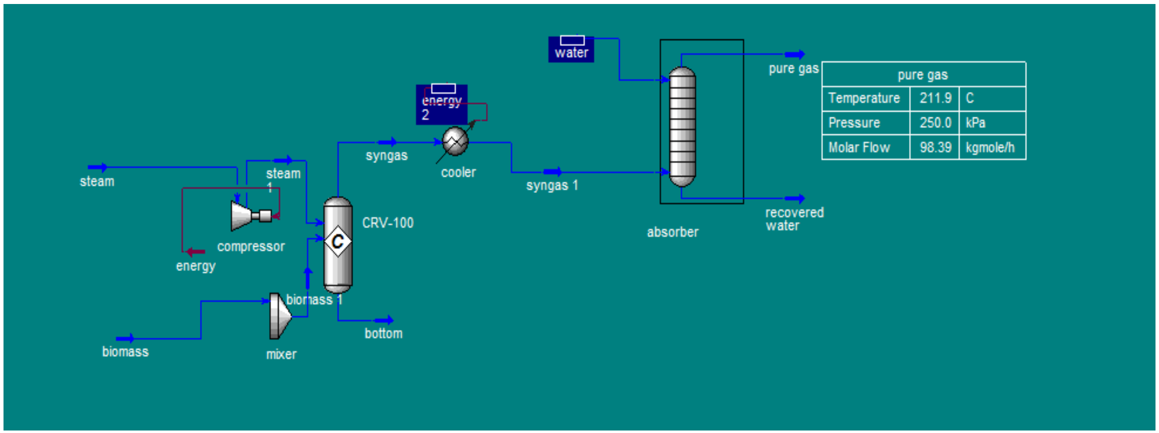
Ash and Char		
Temperature	1000	C
Pressure	101.3	kPa
Molar Flow	0.0000	kgmole/h

Fig. 3.19: Aspen HYSYS® process flowsheet for fluidized bed reactor



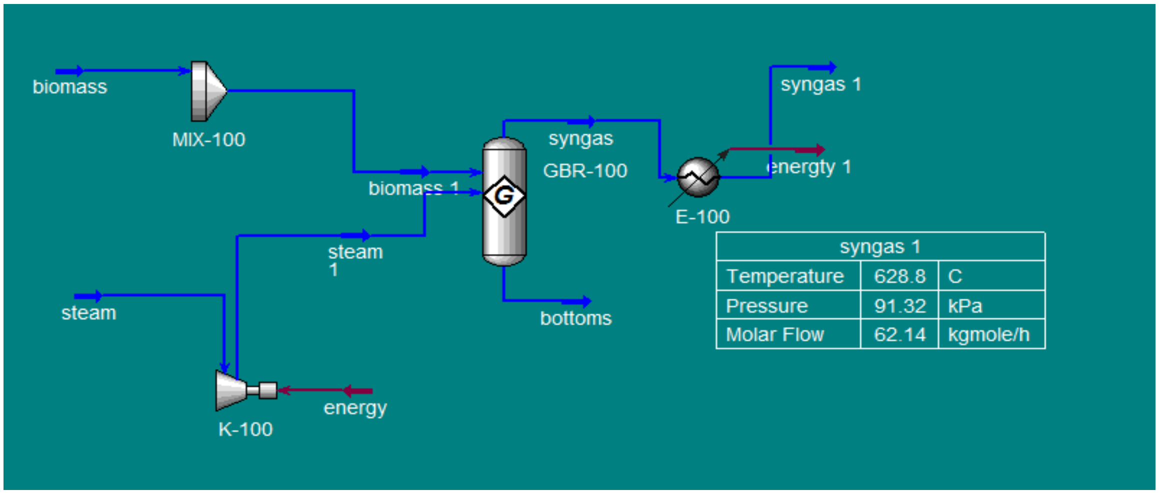
pure gas		
Temperature	211.9	C
Pressure	250.0	kPa
Molar Flow	98.39	kgmole/h

Fig. 3.20: Aspen HYSYS® process flowsheet for fluidized bed reactor



pure gas		
Temperature	211.9	C
Pressure	250.0	kPa
Molar Flow	98.39	kgmole/h

Fig. 3.21: Aspen HYSYS® process flowsheet for fluidized bed reactor



syngas 1		
Temperature	628.8	C
Pressure	91.32	kPa
Molar Flow	62.14	kgmole/h

Fig. 3.22: Aspen HYSYS® process flowsheet for fluidized bed reactor with Gibbs Reactor

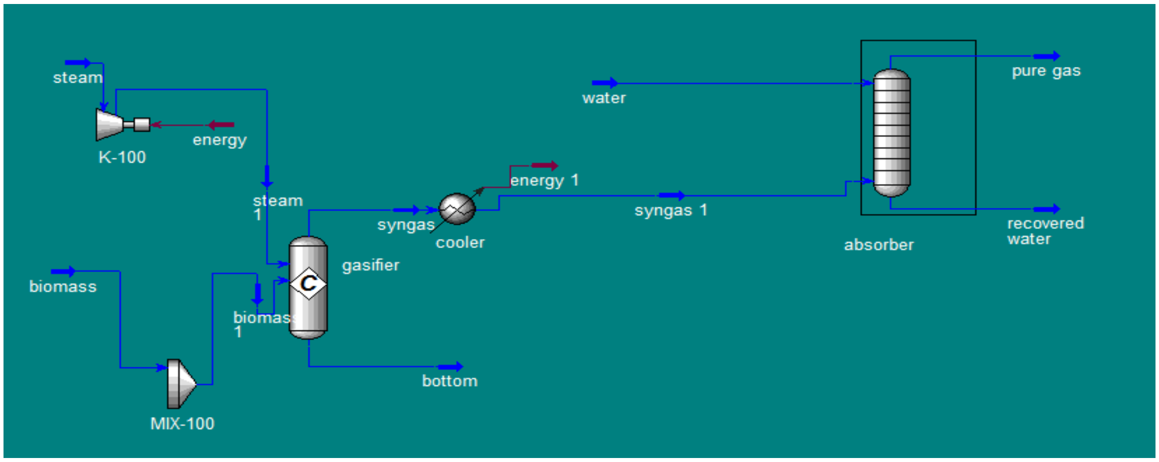


Fig. 3.23: Aspen HYSYS® process flowsheet for fluidized bed reactor

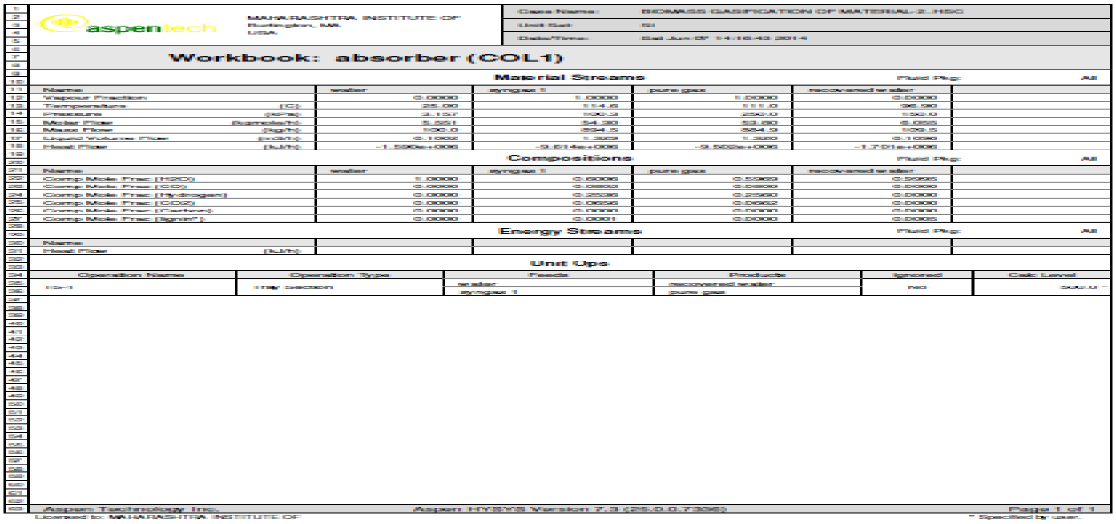
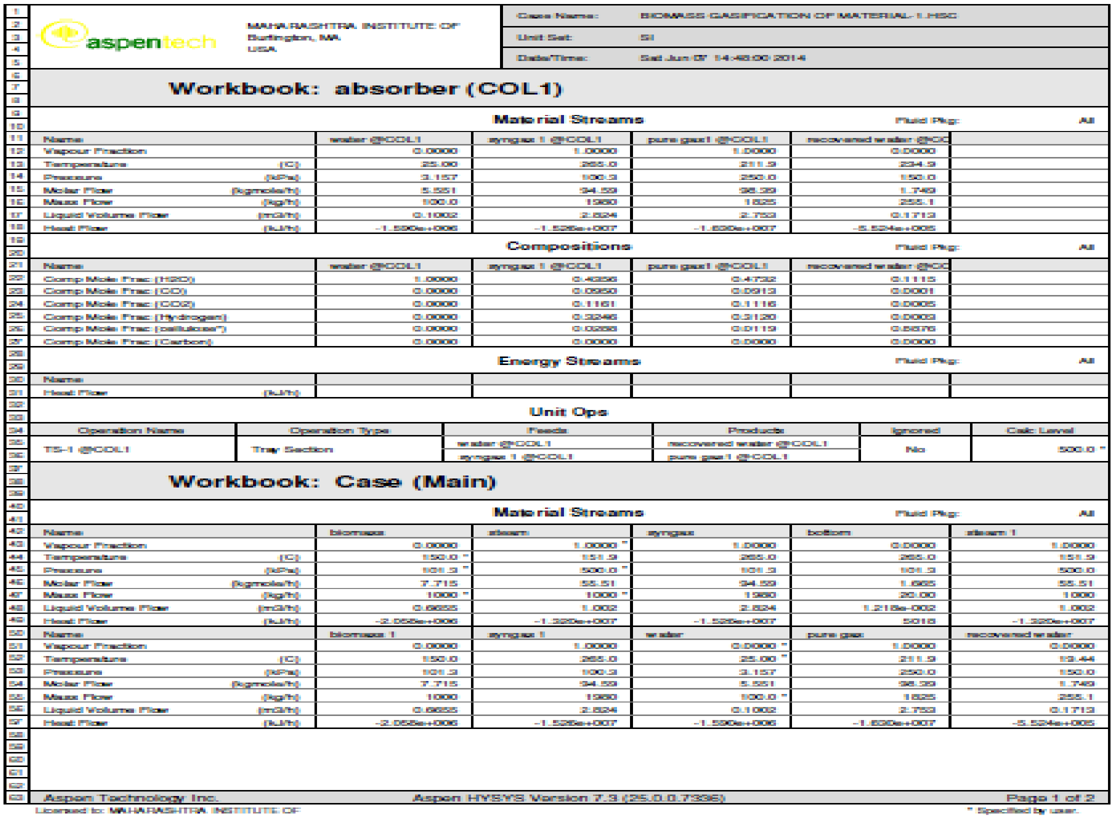

Workbook: absorber (COL1)

Fig. 3.24: Aspen HYSYS® process datasheet for fluidized bed reactor



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USA

Case Name:	BIOMASS GASIFICATION OF MATERIAL- 1.HSC
Unit Set:	SI
Date/Time:	Sat Jun 07 14:48:00 2014

Workbook: absorber (COL1)

Material Streams Fluid Pkg: All

Name		water @COL1	syngas 1 @COL1	pure gas1 @COL1	recovered water @CO
Vapour Fraction		0.0000	1.0000	1.0000	0.0000
Temperature	(C)	25.00	265.0	211.9	234.9
Pressure	(kPa)	3.157	100.3	250.0	150.0
Molar Flow	(kgmole/h)	5.551	94.59	98.39	1.749
Mass Flow	(kg/h)	100.0	1980	1825	255.1
Liquid Volume Flow	(m3/h)	0.1002	2.824	2.753	0.1713
Heat Flow	(kJ/h)	-1.590e+006	-1.526e+007	-1.630e+007	-5.524e+005

Compositions Fluid Pkg: All

Name	water @COL1	syngas 1 @COL1	pure gas1 @COL1	recovered water @CO
Comp Mole Frac (H2O)	1.0000	0.4356	0.4732	0.1115
Comp Mole Frac (CO)	0.0000	0.0950	0.0913	0.0001
Comp Mole Frac (CO2)	0.0000	0.1161	0.1116	0.0005
Comp Mole Frac (Hydrogen)	0.0000	0.3246	0.3120	0.0003
Comp Mole Frac (cellulose*)	0.0000	0.0288	0.0119	0.8876
Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000	0.0000

Energy Streams Fluid Pkg: All

Name						
Heat Flow	(kJ/h)					

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
TS-1 @COL1	Tray Section	water @COL1 syngas 1 @COL1	recovered water @COL1 pure gas1 @COL1	No	500.0 *

Workbook: Case (Main)

Material Streams Fluid Pkg: All

Name		biomass	steam	syngas	bottom	steam 1
Vapour Fraction		0.0000	1.0000 *	1.0000	0.0000	1.0000
Temperature	(C)	150.0 *	151.9	265.0	265.0	151.9
Pressure	(kPa)	101.3 *	500.0 *	101.3	101.3	500.0
Molar Flow	(kgmole/h)	7.715	55.51	94.59	1.665	55.51
Mass Flow	(kg/h)	1000 *	1000 *	1980	20.00	1000
Liquid Volume Flow	(m3/h)	0.6655	1.002	2.824	1.218e-002	1.002
Heat Flow	(kJ/h)	-2.058e+006	-1.320e+007	-1.526e+007	5018	-1.320e+007

Name		biomass 1	syngas 1	water	pure gas	recovered water
Vapour Fraction		0.0000	1.0000	0.0000 *	1.0000	0.0000
Temperature	(C)	150.0	265.0	25.00 *	211.9	13.44
Pressure	(kPa)	101.3	100.3	3.157	250.0	150.0
Molar Flow	(kgmole/h)	7.715	94.59	5.551	98.39	1.749
Mass Flow	(kg/h)	1000	1980	100.0 *	1825	255.1
Liquid Volume Flow	(m3/h)	0.6655	2.824	0.1002	2.753	0.1713
Heat Flow	(kJ/h)	-2.058e+006	-1.526e+007	-1.590e+006	-1.630e+007	-5.524e+005

Aspen Technology Inc. Aspen HYSYS Version 7.3 (25.0.0.7336) Page 1 of 2
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Fig. 3.25: Aspen HYSYS® process datasheet for fluidized bed reactor

Gasification simulation is developed to convert waste into high-value chemicals and fuels (syngas). The H_2: CO ratio achieved in this simulation study is 3.33: 1, whereas it was 1.5:1 in earlier attempts. This is showcased in figures 3.24 and 3.25. The present accomplished H_2: CO ratio is sufficient to use this synthesis gas as a reliable feedstock for F-T Synthesis for manufacturing of various chemicals as well as for power generation using direct feed to gas turbines. The usage of such good quality of synthesis for power generation is already explained in chapter 2.

Considering the limitations over enhancement of H_2: CO ratio in fluidized bed reactor, alternative and innovative design of Horizontal Feeder Gasifier is attempted and presented in chapter 4.

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CHAPTER -4

DESIGN AND OPTIMIZATION OF HORIZONTAL FEEDER GASIFIER

Innovative design of horizontal feeder gasifier is presented in this chapter. Horizontal feeder gasifier is used to reduce the limitations of direct feed injection mechanism. Horizontal feeder gasifier increases the retention time which will help to increase the reaction conversion and reactor efficiency. Introduction of horizontal feeder before the gasifier cleans the feedstock by ash removal and waste particle removal. Preheating of the coal helps in attaining the equilibrium state of reaction in the gasifier reducing chances of non ideality.

A process optimization method has been developed and applied to study the coal gasification for the production of synthesis gas. The boundary definition and the identification of main units are basic steps for the process analysis. Thermodynamic databases, parametric models and steady state simulation using Aspen HYSYS® are the fundamental tools, which are appropriately combined to gain the specific advantages. ***Enhancement of H_2/CO ratio to 3 is a major achievement of the present study.***

Keywords: Limitations of conventional gasifiers, horizontal feeder, screw conveyor, modeling and simulation, optimization

4.1 INTRODUCTION

Gasification is in one sense an old technology, having formed the heart of the town gas industry. With the decline of the town gas industry, gasification became a specialized, niche technology with limited application. After substantial technical development, gasification is now enjoying a considerable renaissance. The reasons for this include the development of new applications such as gas-to-liquids (Fischer-Tropsch) projects, the prospect of increased efficiency and environmental performance including CO_2 capture through the use of Integrated Gasification Combined-Cycle (IGCC) in the power industry [1, 2], as well as the search for an environmentally benign technology to process low-value or waste feedstocks such as refinery residues, petroleum coke, biomass or municipal waste [3].

Biomass and crop residues also have been gasified successfully. Gasification of these materials has many potential benefits over conventional options such as combustion or disposal by incineration [4, 5].

4.2 MECHANISM OF GASIFICATION [3]

In gasifier, as air is passed through the fuel bed, fairly discrete drying, pyrolysis, gasification and oxidation zones develop along the reactor. The location of these zones in the gasifier depends on the relative movement of the fuel and air. These zones are mainly differentiated by the variety of reactions or processes occurring and the temperature regimes at that point. The depth and relative importance of each zone depend on the chemical composition of the feedstock, its moisture content and particle size, the mass flow rate of the gasifying agent, and the temperature.

4.2.1 Drying zone

The drying zone receives its energy through heat transfer from other zones. The rate of drying depends upon the temperature, velocity, and moisture content of the drying gas, as well as the external surface area of the feed material, the internal diffusivity of moisture and the nature of bonding of moisture to that material, and the radioactive heat transfer.

4.2.2 Pyrolysis zone

Heat transfer from the adjacent hot reduction zone causes devolatilization of the feed material. Temperature in the devolatilization zone increases rapidly due to the large temperature difference between the relatively cold feed material and hot gases. The rate of temperature rise is controlled by heat transfer. As feed material pass through this zone, rapid charring and reduction in volume takes place, causing considerable variation in the structure as well as the physical and thermal properties of the material. The products from the devolatilization zone are gases, liquid (tars and oil), and char.

4.2.3 Oxidation zone

In the oxidation zone, physical and chemical changes are inhibited as the oxygen carrier, which is mostly air, is introduced into the fuel bed material. The oxygen burns a portion of the carbon in the fuel material until practically all free carbon is exhausted. Oxygen, however, penetrates the material surface to a small extent because it reacts more readily at the surface with the formed carbon monoxide and hydrogen gases.

4.2.4 Ash cooling zone

In the ash cooling zone, the remaining particles start to cool down faster than particles in other zones. The ash cooling zone formed in fixed bed gasifier protects the grate from intense heat and distributes the air over the bed. Practically no chemical reaction takes place here, although in some fixed bed designs, this zone acts as a filter for the resulting producer gas. However, this zone preheats the incoming air stream in some designs.

4.3 CHEMICAL REACTIONS INVOLVED IN GASIFICATION

Gasification of solid waste with reactive gases such as air, steam, CO_2 and O_2 as well as secondary reactions such as the water gas shift reaction, methanation, tar cracking and reforming of tars and heavy hydrocarbons are normally favored at high temperatures ($>600^oC$). The char-gas reaction ($C-CO_2$ and $C-H_2O$) controls the ultimate conversion of the char, thus their products can dominate the final gas. The composition of the final product gas is dependent on the degree of equilibrium attained by various gas phase reactions.

4.3.1 Heterogeneous reactions

The principle gasification reactions and standard enthalpy change (ΔH_f) are:

$$C + O_2 \longrightarrow CO_2 \qquad -394.4\ \text{kJ/mol} \qquad \ldots..1$$

$$C + \tfrac{1}{2} O_2 \longrightarrow CO \qquad -110.6\ \text{kJ/mol} \qquad \ldots..2$$

$$C + CO_2 \longrightarrow 2\ CO \qquad 173.0\ \text{kJ/mol} \qquad \ldots..3$$

$$C + H_2O_{(g)} \longrightarrow CO + H_2 \qquad 131.4\ \text{kJ/mol} \qquad \ldots..4$$

$$C + 2\ H_2 \longrightarrow CH_4 \qquad -71.0\ \text{kJ/mol} \qquad \ldots..5$$

The combustion reaction occurring in the presence of free oxygen is highly exothermic and very fast. The combustion reactions (1) and (2) provide the energy necessary to sustain the endothermic gasification and other reactions. Other oxidation reactions are also exothermic.

4.3.2 Homogenous reactions

The following gas phase reactions occur in a gasifier to an extent dependent on the operating conditions.

$$CO + H_2O \longrightarrow CO_2 + H_2 \qquad -41.2\ \text{kJ/mol} \qquad \ldots..6$$

$$CO + 3\ H_2 \longrightarrow CH_4 + H_2O \qquad -201.9\ \text{kJ/mol} \qquad \ldots..7$$

$$CO + \tfrac{1}{2} O_2 \longrightarrow CO_2 \qquad -251.0\ \text{kJ/mol} \qquad \ldots..8$$

$$H_2 + \tfrac{1}{2} O_2 \longrightarrow H_2O \qquad -280.0\ \text{kJ/mol} \qquad \ldots..9$$

Other important secondary reactions occur under appropriate conditions (temperature, pressure), which involve decomposition of heavy hydrocarbons and tars to carbon and low molecular gaseous products [6].

4.4 FACTORS INFLUENCING GASIFICATION PROCESS

Several variables seem to affect the gasification process, product composition, and distribution. Some of them are: bed temperature, bed pressure, bed height, fluidization velocity, gasifying medium, equivalence ratio, feed material moisture content, particle size, air to steam ratio, and presence of catalysts. These parameters are quite interrelated and each of them affects the gasification rate, process efficiency, product gas heating value and product distribution.

4.4.1 Bed temperature

The gasification rate as well as the overall performance of the gasifier is temperature dependent. All gasification reactions are normally reversible and the equilibrium point of any of the reactions can be shifted by changing the temperature. The decreasing amount of char indicates that the conversion increases with increase in temperature [7, 8].

4.4.2 Bed pressure

Bed pressure has been reported to have a significant effect on the gasification process.

4.4.3 Bed height

At a given reactor temperature, a longer residence time, due to higher bed height, increases total gas yields.

4.4.4 Equivalence ratio

The equivalence ratio has the strongest influence on the performance of gasifier because it affects bed temperature, gas quality, and thermal efficiency.

4.4.5 Moisture content of feed material

The moisture content of feed material affects reaction temperature due to the energy required to evaporate water in the fuel. Therefore, the gasification process takes place at a lower temperature.

4.4.6 Particle size

The feed particle size significantly affects gasification results. The coarser the particles, the more char and less tar they produce. The rate of thermal diffusion within the particles decreases with increased particle size, thus resulting in a lower heating rate.

4.4.7 Air/steam ratio

Increasing the air to steam ratio increases the gas heating value until it peaks. The results showed that the influence of steam-to-air ratio on char was particularly strong at lower ratios due to the fact that the steam released at the devolatilization stage contributed to the gasification process even in the case when steam was not added [9, 10].

4.5 GASIFICATION PROCESSES [3, 9]

A broad range of reactor types are being used. For most purposes, these reactor types can be grouped into one of three categories: moving-bed gasifier, fluid-bed gasifier, and entrained-flow gasifier. The gasifier in each of these three categories shares certain characteristics that differentiate them from gasifier in other categories.

4.5.1 Moving-bed Gasifier

Moving-bed gasifiers (sometimes called fixed-bed gasifiers) are characterized by a bed in which the coal moves slowly downward under gravity as it is gasified by a blast that is generally, but not always, in a counter-current blast to the coal.

4.5.2 Fluid-bed Gasifier

Fluid-bed Gasifier offers extremely good mixing between feed and oxidant, which promotes both, heat and mass transfer. This ensures an even distribution of material in the bed, and hence a certain amount of only partially reacted fuel is inevitably removed with the ash. This places a limitation on the carbon conversion of fluid-bed processes. The operation of fluid-bed gasifier is generally restricted to temperatures below the softening point of the ash, since ash slagging will disturb the fluidization of the bed. Some attempts [7, 9] have been made to operate into the ash softening zone to promote a limited and controlled agglomeration of ash with the aim of increasing carbon conversion.

4.5.3 Entrained-flow Gasifier

Entrained-flow Gasifier operates with feed and blast in co-current flow. The residence time in these processes is short (a few seconds). The feed is ground to a size of 100 μm or less to promote mass transfer and allow transport in the gas.

Given the short residence time, high temperatures are required to ensure a good conversion, and therefore all entrained-flow gasifiers operate in the slagging range.

4.6 LIMITATIONS ASSOCIATED WITH GASIFICATION PROCESS

Although gasification processes have been highly developed, there are still several limitations. Some of these limitations are related to feedstock characteristics while others are related to the overall design of gasifier.

4.6.1 Moisture Content

The operation of a gasifier is affected by the moisture content of the feedstock. The limiting value of moisture mass fraction varies with fuel energy content. The higher the moisture content of the feedstock, the lower the bed temperature due to the energy required to evaporate the water from the feedstock.

4.6.2 Feeding Systems

The size, shape, density, moisture content and composition of the fuel are the major factors affecting the type of the fuel feed mechanism to be used. Several feeding mechanisms were developed to accommodate the wide variety of feedstock, which includes direct feeding to the bed and over-the-bed feeding.

It is, however, not a common application because of its dependency on the physical properties of the feedstock. This difficulty is addressed in this thesis and remedy suggested.

4.6.3 Ash Deformation Temperature

The deformation temperatures of ash and slag are affected by the composition of the ash and its concentration. Melted ash can clog the grate and ash handling becomes a critical problem.

4.6.4 Particle mixing and segregation

The design of fluidized bed reactors becomes extremely important because both the axial and radial transport of solids within the bed influence gas-solid contacting, thermal gradient and the heat transfer coefficient.

4.6.5 Entrainment and elutriation

Entrainment, elutriation, and carryover are technical terms used interchangeably to describe the ejection of particles from the surface of a bubbling bed, fractionation in the freeboard region and the removal of particles from the fluidized bed unit in the gas stream. Entrainment is expected to be influenced by many factors such as fluidizing gas properties (superficial gas velocity, gas density, viscosity and relative humidity), the solid properties (particle size, particle size distribution and particle density) and other factors (bed diameter, bed depth, gas distribution and internal surfaces) [9].

4.7 ADVANTAGES OF HORIZONTAL FEEDER GASIFIER

Horizontal feeder gasifier is used to reduce the limitations of direct feed injection mechanism. Horizontal feeder gasifier increases the retention time which will help to increase the reaction efficiency. Introduction of horizontal feeder before the gasifier will clean the feedstock by ash removal and waste particle removal. Preheating of the coal helps in attaining the equilibrium state of reaction in the gasifier. Introduction of horizontal feeder into the gasifier system will affect the following parameters:

- Moisture content
- Feeding system
- Ash deformation temperature
- Particle mixing and segregation
- Entrainment and elutriation

Higher moisture content of the feedstock lowers the bed temperature due to the energy required to evaporate the water from the feedstock. Therefore, horizontal feeder gasifier will reduce the energy required to evaporate the moisture content in the feedstock. Gas flow back is minimized in the horizontal feeder gasifier. Horizontal feeder can be used in a wide variety of feedstock's according to their size, shape, density, moisture content and composition which are the major factors in the fuel feed mechanism. Horizontal feeder provides a better and stable retention time in comparison with the direct feeder mechanisms.

4.8 SCHEMATIC DESIGN OF HORIZONTAL FEEDER GASIFIER

A proposed design of horizontal feeder gasifier is shown in the figure 4.1. The design calculations are performed while considering the equipment components shown in the diagram.

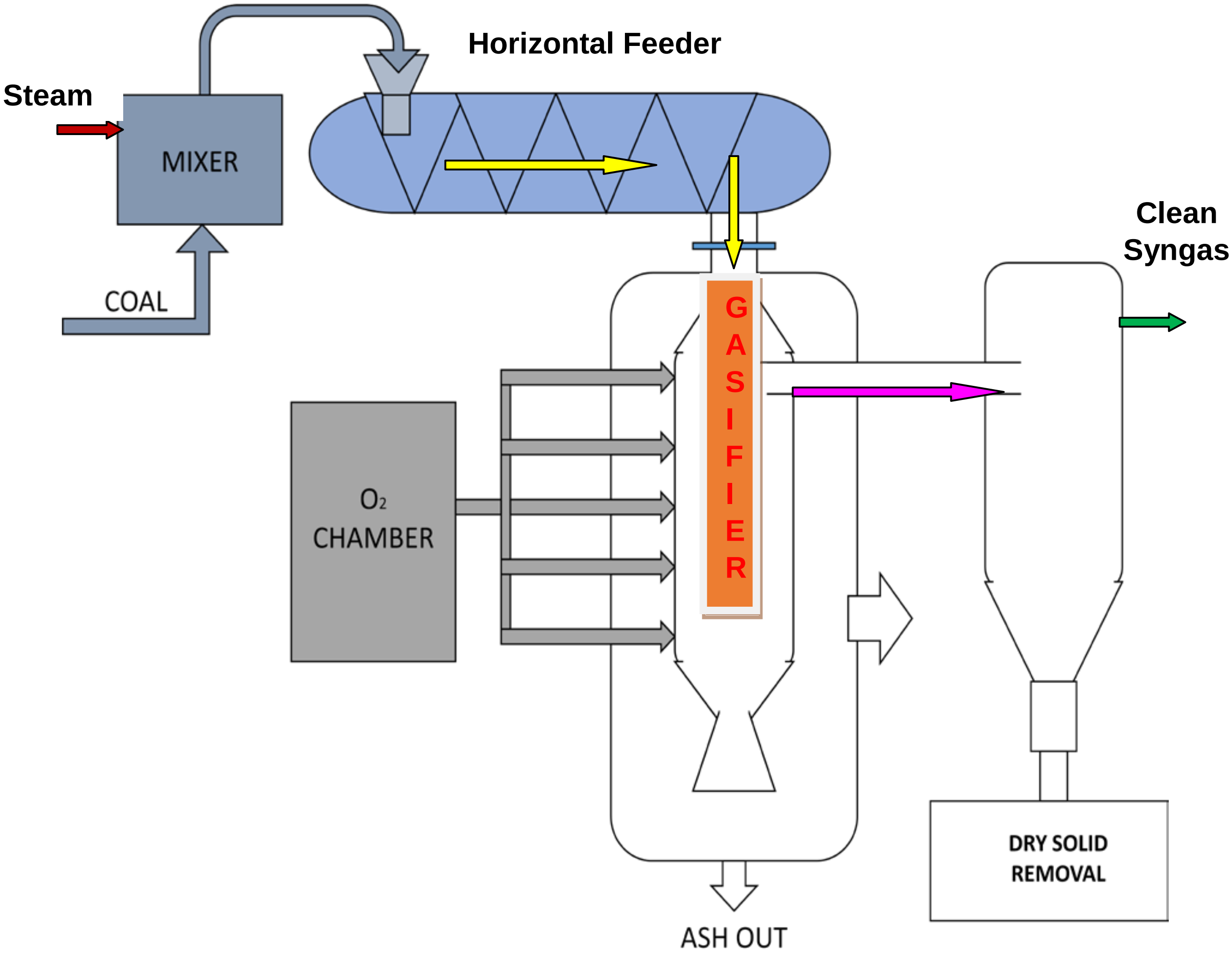


Fig. 4.1: Proposed model of Horizontal Feeder Gasifier

4.9 DESIGN OF HORIZONTAL FEEDER GASIFIER

This section is divided into two parts:

4.9.1 Design of Horizontal Feeder

4.9.2 Design of Gasifier

4.9.1 DESIGN OF HORIZONTAL FEEDER

4.9.1.1 Advantages of Screw Conveyor as Horizontal Feeder

- Screw conveyors are capable of handling a great variety of bulk materials from sluggish to free-flowing.
- Screw conveyors can have multiple inlet and discharge points. Bulk materials can be conveyed and distributed to various locations as required. Slide gates or valves can be added to control the flow into and out of a screw conveyor.
- When a screw conveyor is used as a metering device, it is considered a screw feeder. Screw feeders are used to initiate a material process by metering product from a bin or hopper.

4.9.1.2 Screw Conveyors

Screw conveyors move materials either horizontally, on an incline or vertically. They are used to feed, distribute, collect or mix and can be equipped to either heat or cool while performing this transfer. With the proper cover and gasketing, they are easily made dust or weather tight and rodent proof. Also, they cost less than most other types of conveyors. Some proprietary screw conveyors [10] are ruggedly built and accurately manufactured to assure complete dependability as well as the versatility required to meet a wide range of job assignments.

4.9.1.3 Components of a Screw Conveyor System [10]:

Figure 4.2 shows such a typical commercial screw conveyor which is suitable for present study applications [10].

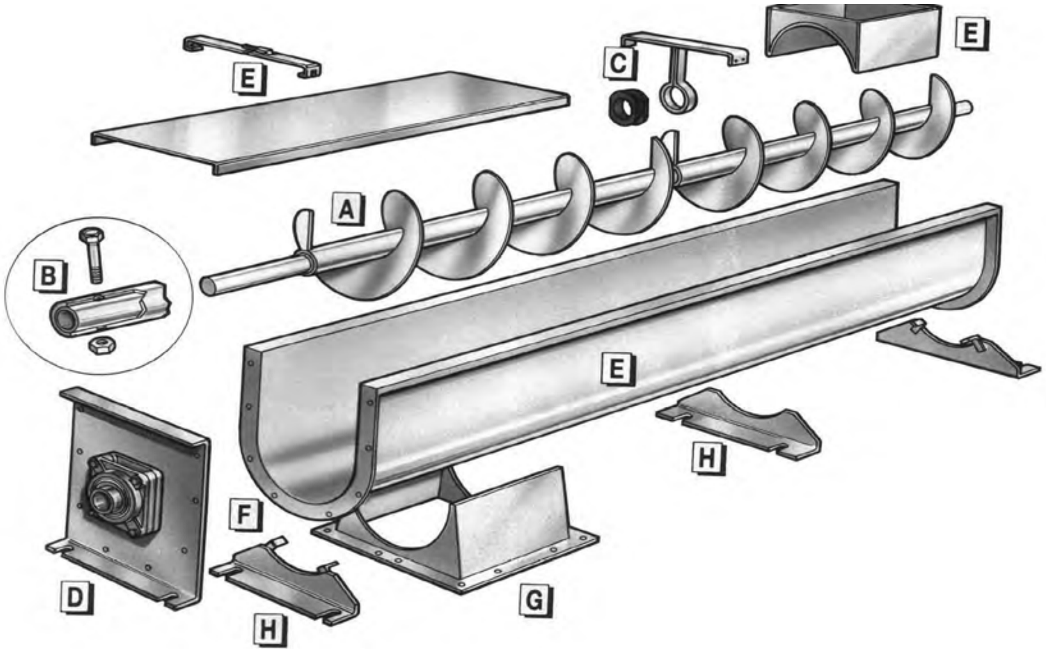


Fig. 4.2: Components of a Screw Conveyor System

The equipment parts indicated by A to H in figure 4.2 are discussed below.

A. **Conveyor Screw:** Compact, manufactured straight and accurate in helicoid, sectional, ribbon and special designs to meet your requirements.

B. **Job-Rated Components:** Selected to meet the performance required. Precisely worked to insure a longer lasting, truer running unit.

   a. **Jig-Drilled Couplings:** Assures easy shaft alignment and assembly. Available with "Redi-Change" clamping key for quick disassembly of conveyor screw.

   b. **Tem-U-Lac Self-Locking Coupling Bolts:** Guards against system damage and costly down-time caused by coupling bolts or nuts working loose.

C. **Hangers and Bearings:** Various styles and bearing materials selected to meet required needs.

D. **Trough Ends:** Several bearing and seal styles are available to match the needs

E. **Troughs, Covers, Clamps and Shrouds:** Ruggedly contracted standard "U" and other styles of troughs including tubular covers, clamps and shrouds available for all applications.

F. **Nu-Weld® Flange:** Continuously welded steel flange holds trough in alignment.

G. **Discharge Spouts:** Any type out of hand, electric, hydraulic or pneumatic powered gates can be used.

H. **Supporting Feet and Saddles:** Align and fasten the trough to the floor or existing structure.

4.9.1.4 Screw Conveyor Design Procedure:

The design algorithm with key steps and elaboration in procedure are provided through figure 4.3 and table 4.1.

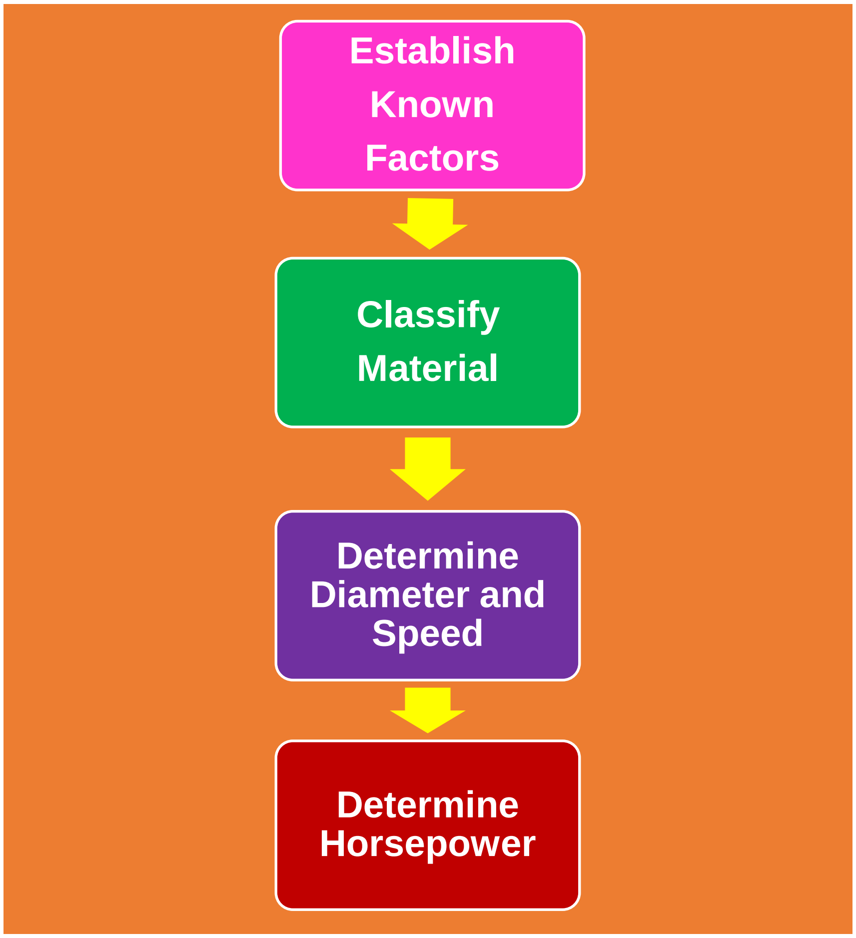


Fig. 4.3: Screw Conveyor design algorithm

Table 4.1: Screw Conveyor Design Procedure

STEP 1	Establish Known Factors	1. Type of material to be conveyed. 2. Maximum size of hard lumps. 3. Percentage of hard lumps by volume. 4. Capacity required, in cu.ft./hr. 5. Capacity required, in lbs./hr. 6. Distance for which material to be conveyed
STEP 2	Classify Material	Classify the material according to the system
STEP 3	Determine Design Capacity	Determine design capacity
STEP 4	Determine Diameter and Speed	Using known capacity required in cu.ft./hr., material classification, and % trough loading determine diameter and speed
STEP 5	Determine Horsepower	Determine Horsepower Factor “Fm” for the material to be conveyed and calculate horsepower by the formula method.

Once the known factors are established, it is essential to classify the material and obtain properties of the material being used. Table 4.2 shows the material properties of raw material selected for present design.

- **Classify Material:**

Table 4.2: Material Properties of Coal

Sl. No.	Material	Maximum particle Size, in	Average weight/ft3	% loading	H.P. Factor
1	Anthracite Coal	-1/2	52.60	30B	0.9
2	Pulverized Coal	-100M	32.35	30A	0.6
3	Sized Coal	-1/2	50	30B	0.6

(Source: Raymond. A. Kulwiec, “Material Handling Handbook” 2nd edition, pp 1028 [11])

Feed rate of the coal is assumed to be 1000 kg /hr (44.143 ft^3/hr)

Bulk density is assumed to be 800 kg/m^3

Length of the screw is assumed to be 24 feet

- **Selection of Conveyor Size and Speed**

In order to determine the size and speed of a screw conveyor, it is necessary first to establish the material code number. It will be seen from what follows that this code number controls the cross-sectional loading that should be used. The various cross-sectional loadings shown in the Capacity Table 4.4 are for use with the standard screw conveyor components and are for use where the conveying operation is controlled with volumetric feeders and where the material is uniformly fed into the conveyor housing and discharged from it. Check lump size limitations before choosing conveyor diameter.

- **Conveyor Speed**

For screw conveyors with screws having standard pitch helical flights, the conveyor speed may be calculated by the formula:

$$\boldsymbol{N = \frac{Required\ capacity, ft^3/hr}{Cubic\ feet\ per\ hour\ at\ 1\ revolution\ per\ minute}}$$

N = revolutions per minute of screw, (but not greater than the maximum recommended speed.)

- **Capacity Table**

The capacity table is provided in figure 4.4 [11], gives the capacities in cubic feet per hour at one revolution per minute for various size screw conveyors for four cross-sectional loadings. Also shown are capacities in cubic feet per hour at the maximum recommended revolutions per minute.

The capacity values given in the table will be found satisfactory for most applications. The maximum capacity of any size screw conveyor for a wide range of materials, and various conditions of loading are obtained from table 4.4 by noting the values of cubic feet per hour at maximum recommended speed.

Table 4.3: Horizontal Screw Conveyor Capacity Table

Degree of Trough Loading	Screw Diameter, in	Maximum RPM	Capacity	
			At maximum RPM	At one RPM
45%	6	165	368	2.23
	9	155	1270	8.20
	12	145	2820	19.40
	14	140	4370	31.20
	16	130	6060	46.70
	18	120	8120	67.60
	20	110	10300	93.70
	24	100	16400	164.00
Non-abrasive material 30%A	6	120	180	1.49
	9	100	545	5.45
	12	90	1160	12.90
	14	85	1770	20.80
	16	80	2500	31.20
	18	75	3380	45.00
	20	70	4370	62.50
	24	65	7100	109.00
Abrasive material 30%B	6	60	90	1.49
	9	55	300	5.45
	12	50	645	12.90
	14	50	1040	20.80
	16	45	1400	31.20
	18	45	2025	45.00
	20	40	2500	62.50
	24	40	4360	109.00

(Source: Raymond. A. Kulwiec, “Material Handling” Handbook 2nd edition, pp 1031 [11])

4.9.1.5 Design Calculations

From table 4.2, the required pulverized coal loading is 30 A.

- Screw diameter = 6 inch
- Cubic feet per hour at 1 revolution = 1.49
- N = Required capacity, cubic feet per hour/cubic feet per hour at 1 revolution per minute

N= 44.143/1.49 = 29.626 RPM

4.9.1.6 Power Requirements

The Power required to operate a horizontal screw conveyor is based on proper installation, uniform and regular feed rate to the conveyor and other design criteria as determined in this book.

The power requirement is the total of the power to overcome friction (P_H) and the power to transport the material at the specified rate (P_N) multiplied by the overload factor F*o* and divided by the total drive efficiency e, or:

The driving power of the loaded screw conveyor is given by:

$$\mathbf{P = P_H + P_N}$$

Where,

P_H = Power necessary for the progress of the material

P_N = Driving power of the screw conveyor at no load

4.9.1.7 Power necessary for the progress of the material P_H:

For a length L of the screw conveyor (feeder), the power PH in kilo watts is the product of the mass flow rate of the material by the length L and an artificial friction coefficient λ, also called the progress resistance coefficient.

$$\mathbf{P_H = I_m. L. \lambda / 367 \quad (kilowatt)}$$

Where,

I_m = Mass flow rate in t/hr

λ = Progress resistance coefficient

Each material has its own coefficient λ. It is generally of the order of 2 to 4. For materials like rock salt etc., the mean value of λ is 2.5. For gypsum, lumpy or dry fine clay, foundry sand, cement, ash, coal, lime, large grain ordinary sand, the mean value of λ is 4.0 [11].

The sliding of the material particles against each other gives rise to internal friction. Other resistance due to grading or shape of the output discharge pattern contributes to the resistance factor. That is why the parameter λ is always higher than that due to pure friction.

4.9.1.8 Drive power of the screw conveyor at no load, P_N:

This power requirement is very low and is proportional to the nominal diameter and length of the screw.

$$P_N = D.L / 20 \text{ (kW)}$$

Where,

D = Nominal diameter of screw in meter

L = Length of screw conveyor in meter

4.9.1.9 Total Power Calculations:

$$P_H = I_m.L.\ \Lambda / 367 \text{ (kW)}$$

$$= 1*3.048*4/367$$

$$P_H = 0.033 \text{ kW}$$

$$P_N = D.\ L / 20$$

$$P_N = 0.06967 \text{ kW}$$

Total Power:

$$P_T = P_H + P_N$$

$$P_T = 0.1033 \text{ kW}$$

4.9.2 DEVELOPMENT OF GASIFIER MODEL

The equilibrium model has been used by many researchers for the analysis of the gasification process. Those models were based on the minimization of Gibbs free energy [14]. This is a constrained optimization problem that generally uses the Lagrange multiplier method. An understanding of some mathematical theories is necessary for solving optimization and non-linear equation problems.

The other kind of equilibrium model is based on equilibrium constant. However, it is important to note that an equilibrium model based on the minimization of Gibbs free energy and one based on equilibrium constants are of the same concept. The amount of oxygen in that model was eliminated by defining it in terms of some components in the producer gas. This model can predict the reaction temperature by knowing the amount of oxygen, and vice versa. To further improve the model, the equilibrium constants were multiplied by the coefficients determined from the comparison of the predicted results with the experimental results [15-16].

4.9.2.1 Thermodynamics study

TO understand the theoretical background of any chemical process, it is necessary to examine both the thermodynamics (i.e. the state to which the process will move under specific conditions of pressure and temperature, given sufficient time) and the kinetics (i.e. what route will it take and how fast will it get there) [17-18].

Table 4.4: Heat Capacities of gases in the Ideal-Gas state, Standard enthalpies and Gibbs free energies of formation at 298.15 K (25^{o}C) [18]

COMPOUNDS	A	B	C	$\Delta H_{f\,298}$	$\Delta G_{f\,298}$
CO	3.376	0.557	0	-110525	-137169
CO_2	5.457	1.045	0	-393509	-394359
H_2	3.249	0.422	0	0	0
H_2O	3.47	1.45	0	-241818	-228572
CH_4	1.702	9.081	-2.164	-74520	-50460
O_2	3.639	0.506	0	0	0
C	1.771	0.771	0	0	0

4.9.2.2 Thermodynamic and Energy Balance

Chemical equilibrium is usually explained either by minimization of Gibbs free energy or by using an equilibrium constant. To minimize the Gibbs free energy, constrained optimization methods are generally used. The present thermodynamic equilibrium model is developed based on the equilibrium constant and not on the Gibbs free energy.

The total Gibbs energy of a closed system at constant T and P must decrease during an irreversible process and that the condition for equilibrium is reached when G_t attains its minimum value. At this equilibrium state,

$$(dG_t)_{T,P} = 0$$

Thus if a mixture of chemical species is not in chemical equilibrium, any reaction that occurs at constant T and P must lead to a decrease in the total Gibbs energy of the system.

$$CO + H_2O \longleftrightarrow CO_2 + H_2$$

To calculate the equilibrium constant for the above reaction from ambient temperature to required temperature:

- First the values of ΔA, ΔB, ΔC of the reaction are determined:

$$\Delta A = A\,(CO_2+H_2) - A\,(CO+H_20)$$
$$= 5.457+3.249 - 3.376 - 3.249$$
$$= 1.86$$
$$\Delta B = -0.00054$$
$$\Delta C = 0$$

- The values of $H_{f\,298}$ and $G_{f\,298}$ for the reaction are calculated from the heat of formation and Gibbs energy formation data

$$\Delta H_{f\,298} = H\,(CO_2+H_2) - H\,(CO+H_20)$$
$$= -393509 + 0 - (-110525 + (-241818))$$
$$\Delta H_{f\,298} = -41166 \text{ kJ/kmol}$$
$$\Delta G_{f\,298} = -28618 \text{ kJ/kmol}$$

$$\Delta H_{f\,298} = \Delta H^{I} + \Delta A*T + \Delta B*T^{2\,+}\ \Delta C*\ T^{3}$$

$$\Delta H^{I} = -41166-(1.86*298+ -0.00054*298^{2})\quad \text{at } T= 298\text{ K}$$

$$\Delta H^{I} = -41696.3\text{ kJ/kmol}$$

$$\Delta G_{f298} = \Delta H^{I} - (\Delta A*T\ \ln T) - (\Delta B*T^{2}/2) - (\Delta C*T^{3}/3) - ART$$

$$A = (\Delta G_{f298} - (\Delta H^{I} - (\Delta A*T\ \ln T) - (\Delta B*T^{2}/2) - (\Delta C*T^{3}/3)))/RT$$

$$A = -6.5435478 \qquad (\text{at } T= 298\text{ K \& } R=8.314)$$

Table 4.5: Thermodynamic parameters obtained for modeling of the gasifier

REACTIONS	**ΔA**	**ΔB**	**ΔC**	**$\Delta H_{F\,298}$**	**$\Delta\ G_{F\,298}$**	**ΔH'**	**A**
$CO + H_2O= CO_2 + H_2$	1.86	-0.00054	0	-41166	-28618	-41696.3	-6.5435
$CH4 + H_2O = CO +3H_2$	7.951	-0.008708	2.164E-06	205813	141863	203811.2	19.6881
$CH_4 + CO_2 = 2CO + 2H_2$	6.091	-0.008168	2.164E-06	246979	170481	245507.5	26.2317
$C + H_2O = CO + H_2$	1.384	-0.001242	0	131293	91403	130935.7	15.0301
$C + 1/2O_2 = CO$	-0.2145	-0.000467	0	-110525	-137169	-110440	10.9435
$C+2\ H_2=CH_4$	-6.567	7.466	-2.164	-74520	-50460	18685003	30546.97

4.9.2.3 Results from Thermodynamic and Kinetic model:

Following are the equations used to calculate the Gibbs free energy and Equilibrium Constant K. The results are tabulated in table 4.6 and demonstrated by figure 4.4.

To calculate $\Delta G_{f\,T}$,

$$\boldsymbol{\Delta G_{f\,T} = \Delta H^{I} - (\Delta A*T\ \ln T) - (\Delta B*T^{2}/2) - (\Delta C*T^{3}/6) - ART}$$

To calculate K,

$$\mathbf{K = -\Delta H^{I}/RT + (\Delta A^{*} \ln T)/R + (\Delta T/2R) + (\Delta C^{*}T^{2}/6R) + A}$$

The values of $\Delta G_{f\,T}$ and K are determined using excel worksheet for temperature from 800 K to 1265 K and results are tabulated in table 4.6.

Table 4.6: Gibbs energy and K values generated for gasification reactions

TEMPERATURE	DEL G(EQ 1)	K1	DEL G(EQ 2)	K2	DEL G(EQ 3)	K3	DEL G (EQ 4	K4	NET DEL G
800	-7947.76	1.19493626	32020.2953	-4.95303132	39968.0553	67.6755435	23963.63397	35.76915393	88004.22453
815	-7339.834	1.08322484	28689.3433	-4.37809325	36029.1773	67.00347807	21944.54575	35.40880632	79323.23227
830	-6732.3001	0.975608	25355.7744	-3.82384438	32088.0745	66.35573903	19925.35487	35.0614982	70636.90371
845	-6125.1489	0.87186635	22019.5846	-3.28918753	28144.73347	65.73102762	17906.06824	34.72653417	61945.23745
860	-5518.3714	0.77179588	18680.7683	-2.77310186	24199.1397	65.12813582	15886.69252	34.4032674	53248.22906
875	-4911.9592	0.67520659	15339.3185	-2.27463637	20251.27768	64.5459386	13867.23414	34.09109542	44545.87118
890	-4305.9037	0.58192134	11995.2272	-1.79290398	16301.1309	63.98338689	11847.69931	33.78945643	35838.1537
905	-3700.197	0.49177477	8648.48495	-1.32707626	12348.68194	63.43950131	9828.094023	33.49782588	27125.06393
920	-3094.8312	0.40461234	5299.08128	-0.87637867	8393.912505	62.91336645	7808.424081	33.21571348	18406.58664
935	-2489.7989	0.32028945	1947.0046	-0.44008623	4436.803471	62.40412578	5788.695097	32.9426604	9682.704295
950	-1885.0926	0.23867068	-1407.7577	-0.01751962	477.3349162	61.91097693	3768.9125	32.67823684	953.397066
965	-1280.7054	0.15962905	-4765.2193	0.391958381	-3484.51383	61.43316754	1749.08155	32.42203974	-7781.357
980	-676.63044	0.08304537	-8125.3946	0.788946074	-7448.76417	60.96999138	-270.792657	32.1736907	-16521.5819
995	-72.861001	0.00880769	-11488.299	1.174005803	-11415.4382	60.52078492	-2290.70518	31.93283422	-25267.3035
1010	530.609321	-0.0631893	-14853.949	1.547666603	-15384.5586	60.08492408	-4310.65123	31.69913587	-34018.5498
1025	1133.78677	-0.1330447	-18222.362	1.910426639	-19356.1488	59.66182143	-6330.62616	31.47228087	-42775.3502
1040	1736.67741	-0.2008518	-21593.555	2.262755425	-23330.2327	59.25092348	-8350.62546	31.25197258	-51537.736
1055	2339.28714	-0.2666988	-24967.548	2.605095857	-27306.8349	58.85170827	-10370.6447	31.03793126	-60305.7402
1070	2941.62167	-0.3306686	-28344.359	2.937866079	-31285.9804	58.4636832	-12390.6797	30.82989286	-69079.3973
1085	3543.68656	-0.3928399	-31724.008	3.261461185	-35267.6949	58.08638295	-14410.7263	30.62760797	-77858.743
1100	4145.48723	-0.4532866	-35106.517	3.576254793	-39252.0045	57.71936763	-16430.7805	30.43084076	-86643.815
1115	4747.02893	-0.512079	-38491.907	3.882600481	-43238.9357	57.3622211	-18450.8383	30.23936813	-95434.6518
1130	5348.31679	-0.5692836	-41880.199	4.18083312	-47228.5157	57.01454933	-20470.8959	30.05297882	-104231.294
1145	5949.35578	-0.6249632	-45271.416	4.471270093	-51220.7718	56.67597901	-22490.9497	29.87147268	-113033.782
1160	6550.15075	-0.6791775	-48665.581	4.754212424	-55215.7322	56.34615618	-24510.996	29.69465988	-121842.159
1175	7150.70644	-0.7319831	-52062.719	5.029945822	-59213.425	56.02474499	-26531.0313	29.52236033	-130656.468
1190	7751.02745	-0.7834338	-55462.852	5.298741641	-63213.8791	55.71142657	-28551.0522	29.354403	-139476.755
1205	8351.11827	-0.8335805	-58866.005	5.560857775	-67217.1235	55.40589796	-30571.0553	29.19062541	-148303.066
1220	8950.98328	-0.8824719	-62272.204	5.81653948	-71223.1878	55.10787113	-32591.0374	29.03087307	-157135.446
1235	9550.62675	-0.9301541	-65681.475	6.066020142	-75232.1017	54.81707209	-34610.9954	28.87499899	-165973.945
1250	10150.0528	-0.9766709	-69093.843	6.309521989	-79243.8955	54.53324003	-36630.926	28.72286327	-174818.611
1265	10749.2656	-1.0220644	-72509.334	6.547256745	-83258.5997	54.25612655	-38650.8262	28.57433262	-183669.494
1280	11348.2691	-1.0663742	-75927.976	6.779426253	-87276.245	53.9854949	-40670.6933	28.42928004	-192526.645
1295	11947.0671	-1.1096385	-79349.796	7.006223039	-91296.8626	53.72111934	-42690.5241	28.28758438	-201390.115
1310	12545.6634	-1.1518935	-82774.821	7.227830844	-95320.484	53.46278451	-44710.316	28.14913009	-210259.957
1325	13144.0617	-1.1931738	-86203.079	7.444425127	-99347.1408	53.21028482	-46730.0661	28.01380682	-219136.224
1340	13742.2657	-1.2335124	-89634.599	7.656173519	-103376.865	52.96342389	-48749.7718	27.88150919	-228018.97
1355	14340.2789	-1.272941	-93069.41	7.863236261	-107409.689	52.72201408	-50769.4304	27.75213648	-236908.25
1370	14938.1047	-1.3114898	-96507.54	8.065766604	-111445.645	52.485876	-52789.0394	27.6255924	-245804.12
1385	15535.7465	-1.3491876	-99949.019	8.263911189	-115484.766	52.25483802	-54808.5963	27.50178481	-254706.634
1400	16133.2076	-1.386062	-103393.88	8.4578104	-119527.084	52.02873591	-56828.0986	27.38062555	-263615.852
1415	16730.4914	-1.4221396	-106842.14	8.647598693	-123572.634	51.80741242	-58847.5438	27.26203019	-272531.829
1430	17327.6008	-1.4574457	-110293.85	8.833404906	-127621.448	51.59071692	-60866.9297	27.14591785	-281454.625
1445	17924.5391	-1.4920045	-113749.02	9.015352554	-131673.561	51.37850505	-62886.2539	27.03221101	-290384.297
1460	18521.3093	-1.5258393	-117207.7	9.193560097	-135729.005	51.17063839	-64905.5141	26.92083535	-299320.907
1475	19117.9143	-1.5589726	-120669.9	9.368141197	-139787.816	50.96698417	-66924.7082	26.81171956	-308264.512
1490	19714.357	-1.5914256	-124135.67	9.539204963	-143850.027	50.767415	-68943.8339	26.70479522	-317215.175
1505	20310.6405	-1.6232189	-127605.03	9.70685617	-147915.673	50.57180856	-70962.8892	26.59999663	-326172.955

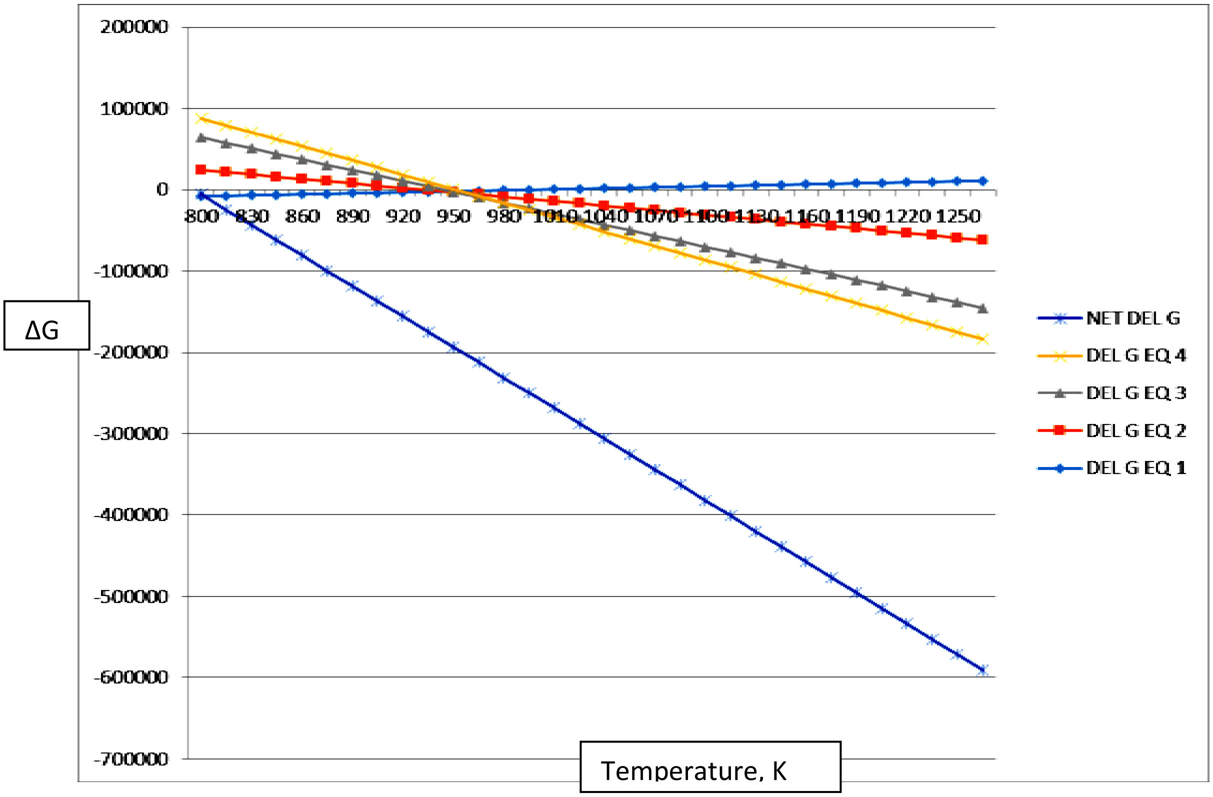


Fig. 4.4: Plot of Temperature and ΔG for four reactions in gasification

From the above figure, we can conclude that operating temperature of the gasifier should be above 980 K to achieve maximum conversion in the gasifier. At this temperature, Gibbs free energy falls negative and thus reaction achieves equilibrium. This equilibrium will now be disturbed by kinetic model and the equilibrium will be shifted so as to provide maximum conversion and products..

4.9.2.4 Thermodynamic equilibrium

In general, the forward and the reverse reactions take place simultaneously and at different rates. For any given temperature, these reaction rates are proportional to the quantity of reactants available to drive the reaction in the direction under consideration. If we take the CO shift reaction as an example, the forward reaction rate, R_f , is proportional to the molar concentrations of CO and H_2O per unit volume, or

$$R_f = k_f \cdot [CO] \cdot [H_2O]$$

where the constant of proportionality, k_f , is temperature-dependent.

Similarly, for the reverse reaction,

$$Rr = kr \cdot [CO_2] \cdot [H_2]$$

Over a period of time, these two reaction rates will tend to reach a common value and the gas composition will have reached a state of equilibrium. Under these circumstances,

$$K\boldsymbol{p} = \frac{\boldsymbol{k_f}}{\boldsymbol{k_r}} = \frac{[\boldsymbol{CO_2}].[\boldsymbol{H_2}]}{[\boldsymbol{CO}].[\boldsymbol{H_2O}]}$$

Where *Kp* is the temperature-dependent equilibrium constant for the CO shift reaction.

Assuming ideal gases this can also be expressed as:

$$Kp = \frac{p_{CO_2}.p_{H_2}}{p_{CO}.p_{H_2O}} = \frac{v_{CO_2}.v_{H_2}}{v_{CO}.v_{H_2O}}$$

Where p_{CO} is the partial pressure and v_{CO} is the volume fraction of CO in the gas, and so on.

Similarly, the equilibrium constants for the other reactions can be expressed as:

$$Kp = \frac{p^2{}_{CO}}{p_{CO_2}} = \frac{(v_{CO})^2}{v_{CO_2}}.p$$

For the reaction 4,

$$Kp = \frac{p_{CO}.p_{H_2}}{p_{H_2O}} = \frac{v_{CO}.v_{H_2}}{v_{H_2O}}.p$$

$$Kp = \frac{p_{CH_4}}{p_{H_2}} = \frac{v_{CH_4}}{v^2{}_{H_2}}.\frac{1}{p}$$

For the methanation reaction and for the reforming reaction, where *p* is the total absolute pressure of the gas:

$$Kp = \frac{p_{CO} \cdot p^3{}_{H_2}}{p_{CH_4} \cdot p_{H_2O}} = \frac{v_{CO} \cdot v^3{}_{H_2}}{v_{CH_4} \cdot v_{H_2O}} \cdot p^2$$

The temperature dependency of these equilibrium constants can be derived from fundamental data, but is usually expressed as a correlation of the type

$$\ln(Kp, T) = \ln(Kp, T_0) + f(T)$$

where *T* is the absolute temperature in Kelvin.

4.9.2.5 Material balance

To develop the model, the chemical formula of feedstock is defined as $CH_XO_YN_Z$, where x, y, and z are the number of atoms of hydrogen, oxygen, and Nitrogen per number of atom of carbon in the feedstock, respectively;

For Indian Coal, $CH_{1.02}O_{0.15}$, is chosen as the molecular formula.

The global gasification reaction can be written as follows:

$$CH_{1.02}O_{0.15} + w\,H_2O + m\,O_2 + 3.76\,m\,N_2 \longrightarrow x_1\,H_2 + x_2\,CO + x_3\,CO_2 + x_4\,H_2O$$

W is the amount of moisture per kmol of feedstock; and m is the amount of oxygen per kmol of feedstock. x_1, x_2, x_3, x_4 are the amount of H_2, CO, CO_2, H_2O per kmol of feedstock.

- Carbon Balance
    - $x_2+x_3-1=0$
- Oxygen Balance
    - $x_2+x_3+x_4=w+m+0.15$
- Hydrogen Balance
    - $x_1+x_4-1.02-w=0$

4.9.2.6 Mathematical modeling of Gasifier

From the Degrees of Freedom (DOF) analysis, five equations are required to find the five unknown species of the producer gas. Those equations are generated using mass balance and equilibrium constant relationships. Considering the global gasification reaction, the first equation is formulated by balancing each chemical element.

- Carbon balance:

  $x_2+x_3-1=0$

- Oxygen balance
  $x_2+x_3+x_4=w+m+0.15$
- Hydrogen balance

  $x_1+ x_4 -1.02-w=0$

From equilibrium:

$$Kp = \frac{{p^2}_{CO}}{p_{CO_2}} = \frac{(v_{CO})^2}{v_{CO_2}}.p$$

- $K_6 = [x_2]^2/[x_3]$

$$Kp = \frac{p_{CO}.p_{H_2}}{p_{H_2O}} = \frac{v_{CO}.v_{H_2}}{v_{H_2O}}.p$$

- $K_4 = [x_2 * x_1] / [w]$

Assumptions:

- W is assumed to be 1
- Flow rate of coal is at 1000 kg/hr
- No methane formation is taking place at outlet gas

The effect of temperature on composition of the product gas is presented in table 4.7. The results show that 1400 K appears to be the optimum temperature for best possible composition of the synthesis gas.

Table 4.7: Variation of mole fraction of product gas with temperature

	$C + H_2O = CO + H_2$	$C + CO_2 = 2C0$					
TEMPERATURE	K4	k6	X2	X3	X4	X1	M
1240	28.82387843	0.01237679	0.10523463	0.89476537	0.00552926	1.51447074	0.35552926
1245	28.77316816	0.05515515	0.208887376	0.791112624	0.01095536	1.50904464	0.36095536
1250	28.72286327	0.09758974	0.267386535	0.732613465	0.01401946	1.50598054	0.36401946
1255	28.67295889	0.13968468	0.310371589	0.689628411	0.01627711	1.50372289	0.36627711
1260	28.62345024	0.18144401	0.344794344	0.655205656	0.01809179	1.50190821	0.36809179
1265	28.57433262	0.22287171	0.373630798	0.626369202	0.01961861	1.50038139	0.36961861
1270	28.52560141	0.2639717	0.398478062	0.601521938	0.02094057	1.49905943	0.37094057
1275	28.47725204	0.30474783	0.420308931	0.579691069	0.02210808	1.49789192	0.37210808
1280	28.42928004	0.34520392	0.439766682	0.560233318	0.0231544	1.4968456	0.3731544
1285	28.38168098	0.38534368	0.457302096	0.542697904	0.02410276	1.49589724	0.37410276
1290	28.33445052	0.4251708	0.473245012	0.526754988	0.02497015	1.49502985	0.37497015
1295	28.28758438	0.46468891	0.487845004	0.512154996	0.02576936	1.49423064	0.37576936
1300	28.24107836	0.50390157	0.501296034	0.498703966	0.02651033	1.49348967	0.37651033
1305	28.19492829	0.5428123	0.513752176	0.486247824	0.02720095	1.49279905	0.37720095
1310	28.14913009	0.58142454	0.525338075	0.474661925	0.02784756	1.49215244	0.37784756
1315	28.10367975	0.61974172	0.536156131	0.463843869	0.02845538	1.49154462	0.37845538
1320	28.05857329	0.65776718	0.546291589	0.453708411	0.02902874	1.49097126	0.37902874
1325	28.01380682	0.69550422	0.555816233	0.444183767	0.02957129	1.49042871	0.37957129
1330	27.9693765	0.7329561	0.564791118	0.435208882	0.03008612	1.48991388	0.38008612
1335	27.92527853	0.77012604	0.573268639	0.426731361	0.03057589	1.48942411	0.38057589
1340	27.88150919	0.80701717	0.581294111	0.418705889	0.03104287	1.48895713	0.38104287
1345	27.83806481	0.84363262	0.588907005	0.411092995	0.03148906	1.48851094	0.38148906
1350	27.79494176	0.87997545	0.596141924	0.403858076	0.03191621	1.48808379	0.38191621
1355	27.75213648	0.91604868	0.60302937	0.39697063	0.03232584	1.48767416	0.38232584
1360	27.70964546	0.95185528	0.60959638	0.39040362	0.03271933	1.48728067	0.38271933
1365	27.66746524	0.98739818	0.615867029	0.384132971	0.03309786	1.48690214	0.38309786
1370	27.6255924	1.02268028	0.621862851	0.378137149	0.03346254	1.48653746	0.38346254
1375	27.58402358	1.05770442	0.627603185	0.372396815	0.03381432	1.48618568	0.38381432
1380	27.54275547	1.0924734	0.633105461	0.366894539	0.03415407	1.48584593	0.38415407
1385	27.50178481	1.12698999	0.638385448	0.361614552	0.03448259	1.48551741	0.38448259
1390	27.46110837	1.16125692	0.643457455	0.356542545	0.03480058	1.48519942	0.38480058
1395	27.420723	1.19527686	0.648334504	0.351665496	0.03510871	1.48489129	0.38510871
1400	27.38062555	1.22905247	0.653028483	0.346971517	0.03540756	1.48459244	0.38540756
1405	27.34081295	1.26258636	0.65755027	0.34244973	0.03569767	1.48430233	0.38569767
1410	27.30128216	1.2958811	0.661909844	0.338090156	0.03597955	1.48402045	0.38597955
1415	27.26203019	1.32893922	0.666116382	0.333883618	0.03625364	1.48374636	0.38625364
1420	27.22305408	1.36176323	0.670178341	0.329821659	0.03652037	1.48347963	0.38652037
1425	27.18435093	1.39435559	0.674103529	0.325896471	0.03678012	1.48321988	0.38678012
1430	27.14591785	1.42671874	0.677899172	0.322100828	0.03703326	1.48296674	0.38703326
1435	27.10775203	1.45885506	0.681571967	0.318428033	0.03728012	1.48271988	0.38728012
1440	27.06985067	1.49076693	0.685128136	0.314871864	0.03752101	1.48247899	0.38752101
1445	27.03221101	1.52245667	0.688573461	0.311426539	0.03775621	1.48224379	0.38775621
1450	26.99483036	1.55392659	0.691913334	0.308086666	0.03798599	1.48201401	0.38798599
1455	26.95770602	1.58517895	0.695152783	0.304847217	0.0382106	1.4817894	0.3882106
1460	26.92083535	1.61621598	0.698296505	0.301703495	0.03843027	1.48156973	0.38843027
1465	26.88421576	1.6470399	0.701348899	0.298651101	0.03864522	1.48135478	0.38864522

4.9.2.7 Effect of temperature

The temperature is generally selected on the basis of the ash properties. It is placed below the softening point of the ash for fluid-bed and dry ash moving-bed gasifier and above the melting point for slagging gasifier. For coals with very high ash melting points, it is often advantageous to add flux to the coal feed in order to lower the ash melting point. Generally, gasifying at very high temperatures will increase the oxygen consumption of a gasification process and will reduce the overall process efficiency [12].

For process control purposes, where ratios between fuel, oxygen and/or steam are known, the temperature can be calculated. This is an important aspect, as temperatures in slagging gasifier can only be measured with great difficulty and are generally not very trustworthy. Since most modern gasification processes operate at pressures of 30 bar or higher, temperatures of above 1300 K are required in order to produce a synthesis gas with a low methane content [2].

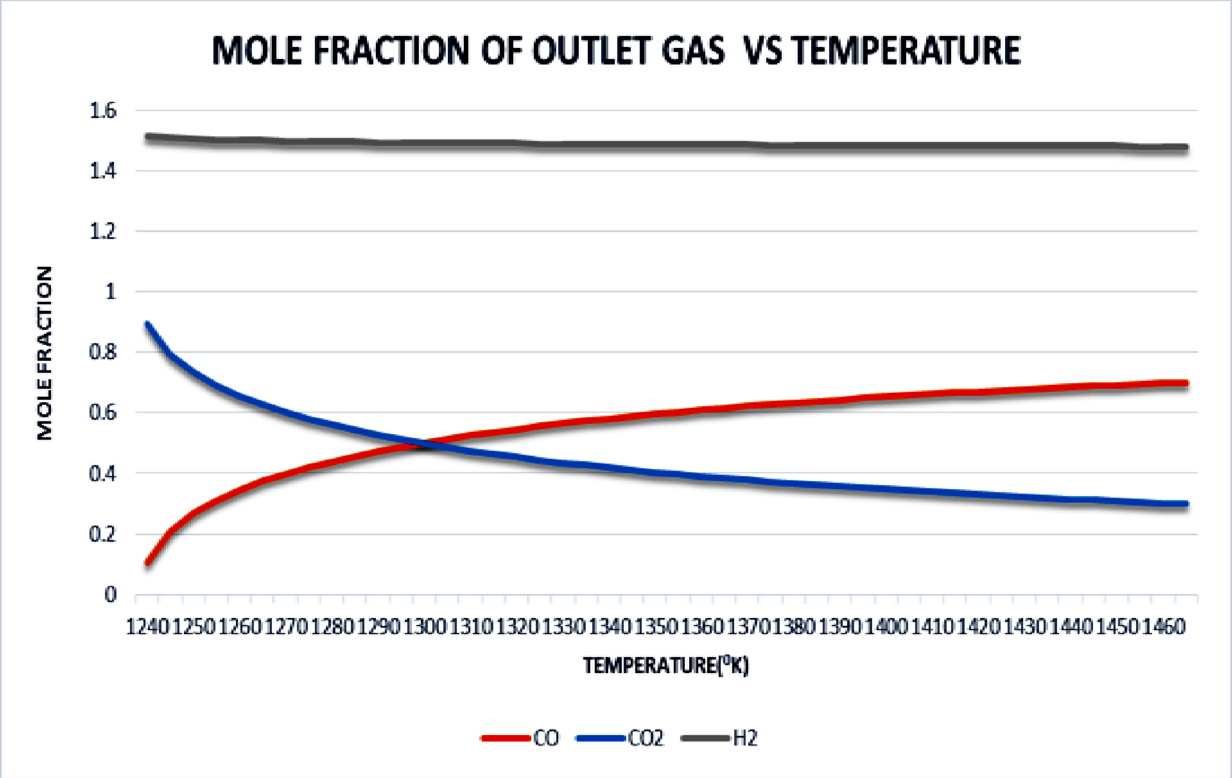


Fig 4.5: Plot of mole fraction of outlet gas and temperature

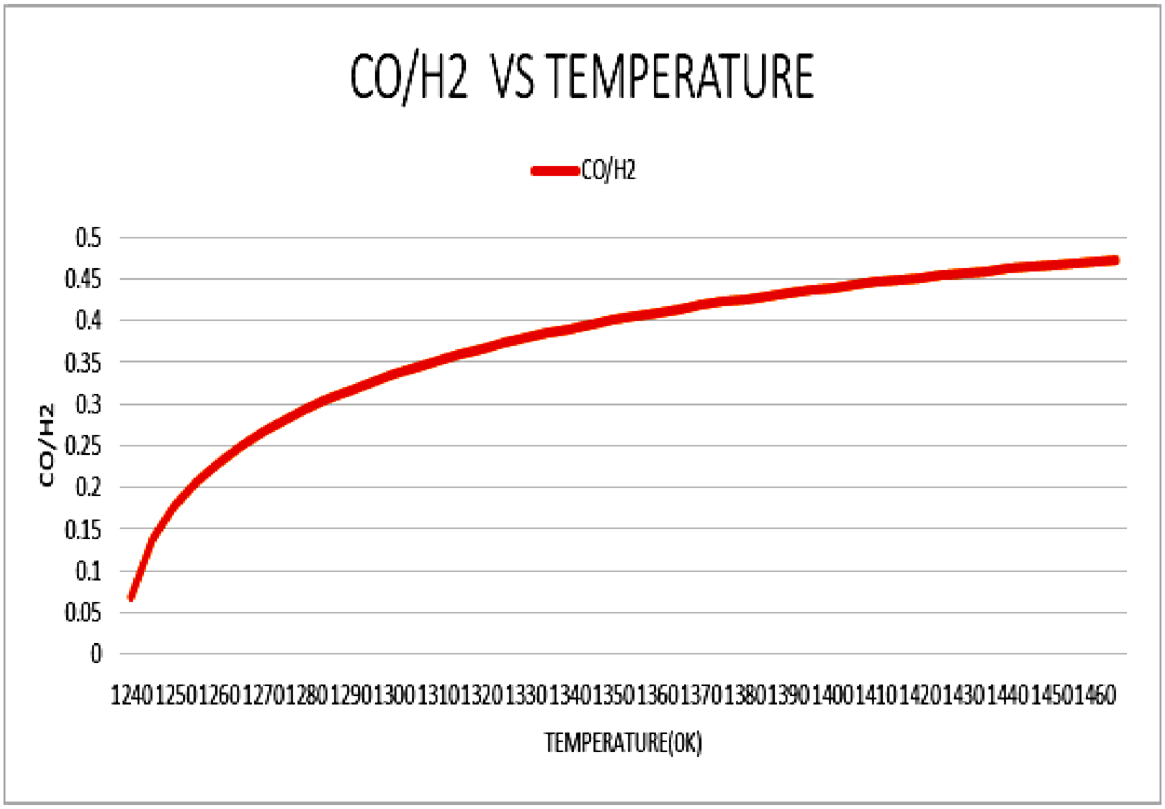


Fig 4.6: Effect of temperature on CO/H_2 mole fraction ratio

From the above two graphs, we can conclude that operating temperature of the gasifier should be 1290 K to 1330 K. This gives minimum CO_2 production along with appreciable low CO/H_2 ratio, meaning high quality of synthesis gas.

For this optimized condition, the mass flowrates of reactants and products are calculated and tabulated in table 4.8.

Table 4.8: Flow rate of outlet gas (kg/hr)

COAL	w H2O	m O2	3.76 m n2	x1 H2	X2 CO	x3 CO2	x4 H20
1000	592.1052632	748.4826562	2462.507939	199.2724656	193.8532654	2590.110282	0.099526711
1000	592.1052632	759.9060181	2500.0908	198.5585054	384.7925352	2290.062858	0.197196455
1000	592.1052632	766.3567496	2521.313706	198.1553347	492.554143	2120.723189	0.252350209
1000	592.1052632	771.1097021	2536.95092	197.8582752	571.7371372	1996.292769	0.292987953
1000	592.1052632	774.9300845	2549.519978	197.6195013	635.1474751	1896.647953	0.325652223
1000	592.1052632	778.1444427	2560.095216	197.4186039	688.2672587	1813.174007	0.353134985
1000	592.1052632	780.9275117	2569.251514	197.2446621	734.0385362	1741.247714	0.376930225
1000	592.1052632	783.3854305	2577.338066	197.0910422	774.2532943	1678.053094	0.397945431
1000	592.1052632	785.5882034	2584.585189	196.9533689	810.0965202	1621.728025	0.416779139
1000	592.1052632	787.5847651	2591.153877	196.8285838	842.3985979	1570.967617	0.433849741
1000	592.1052632	789.4108377	2597.161656	196.7144542	871.7671279	1524.81707	0.449462663
1000	592.1052632	791.09339	2602.697253	196.6092947	898.66185	1482.553935	0.463848485
1000	592.1052632	792.6533366	2607.829478	196.511798	923.4400618	1443.616745	0.477186028
1000	592.1052632	794.1072577	2612.612878	196.420928	946.3855872	1407.559491	0.489617053
1000	592.1052632	795.4685401	2617.091497	196.3358478	967.7280327	1374.021362	0.501256018
1000	592.1052632	796.7481615	2621.301451	196.2558715	987.65603	1342.705938	0.512196781
1000	592.1052632	797.9552443	2625.272754	196.1804288	1006.326611	1313.366453	0.522517339
1000	592.1052632	799.0974574	2629.030635	196.1090405	1023.872007	1285.795116	0.532283261
1000	592.1052632	800.1813133	2632.596521	196.0412995	1040.404691	1259.815185	0.541550228
1000	592.1052632	801.2123917	2635.988769	195.9768571	1056.021176	1235.274993	0.550365949
1000	592.1052632	802.1955117	2639.223234	195.9154121	1070.80494	1212.043364	0.558771625
1000	592.1052632	803.1348652	2642.313706	195.8567025	1084.828694	1190.006037	0.566803097
1000	592.1052632	804.0341215	2645.27226	195.800499	1098.156175	1169.062853	0.574491739
1000	592.1052632	804.8965118	2648.109524	195.7465996	1110.843576	1149.125508	0.581865176
1000	592.1052632	805.7248962	2650.834909	195.6948256	1122.9407	1130.115742	0.588947863
1000	592.1052632	806.5218189	2653.456784	195.6450179	1134.491896	1111.963862	0.595761552
1000	592.1052632	807.2895529	2655.982629	195.5970345	1145.536832	1094.607535	0.602325677
1000	592.1052632	808.0301373	2658.419152	195.550748	1156.11113	1077.990781	0.608657674
1000	592.1052632	808.7454086	2660.772394	195.5060435	1166.246902	1062.063139	0.614773244
1000	592.1052632	809.4370262	2663.047816	195.4628174	1175.973194	1046.778965	0.620686574
1000	592.1052632	810.1064947	2665.250368	195.4209757	1185.316364	1032.096841	0.62641053
1000	592.1052632	810.7551825	2667.38455	195.3804327	1194.300403	1017.979066	0.63195681
1000	592.1052632	811.3843374	2669.45447	195.3411105	1202.947206	1004.391232	0.637336085
1000	592.1052632	811.9951007	2671.463881	195.3029378	1211.276813	991.3018496	0.642558111
1000	592.1052632	812.5885187	2673.416226	195.2658492	1219.307608	978.6820298	0.647631835
1000	592.1052632	813.1655526	2675.314668	195.2297845	1227.056494	966.5052093	0.652565474
1000	592.1052632	813.7270879	2677.162119	195.1946886	1234.539049	954.7469087	0.657366601
1000	592.1052632	814.2739418	2678.961269	195.1605102	1241.769658	943.3845225	0.662042202
1000	592.1052632	814.80687	2680.714602	195.1272022	1248.761632	932.3971348	0.666598739
1000	592.1052632	815.3265728	2682.424424	195.0947208	1255.527308	921.7653574	0.671042197
1000	592.1052632	815.8336999	2684.092873	195.0630253	1262.078145	911.4711863	0.675378134
1000	592.1052632	816.3288557	2685.721935	195.0320781	1268.424797	901.4978751	0.679611716
1000	592.1052632	816.8126028	2687.313463	195.0018439	1274.577194	891.8298224	0.683747754
1000	592.1052632	817.2854663	2688.869184	194.9722899	1280.544599	882.4524716	0.687790737
1000	592.1052632	817.7479364	2690.390711	194.9433856	1286.335668	873.3522209	0.691744856
1000	592.1052632	818.2004717	2691.879552	194.9151021	1291.958499	864.5163437	0.695614033

4.10 SIMULATION AND OPTIMIZATION

4.10.1 SIMULATION OF THE PROCESS

This process is modeled using Aspen HYSYS®, the commercially available software capable of handling coal and sorbent solid components. This software can handle the rigorous material and energy balances of the process. Figure 4.7 demonstrates the simulation flowsheet built in Aspen HYSYS® along with equipment components. The horizontal feeder reactor is not available in the simulator as an inbuilt model. Equilibrium Reactor is modeled with necessary changes in design specifications. This is an outcome of the present study, which is not done before. Figure 4.11 summarizes the simulation results for the most important streams in the base case using a basis of 1000 kg of coal feed per hour.

4.10.2 Simulating the Coal Feed Stream

Although Aspen HYSYS® has a component named COAL in its solids databank, it is not the component used in the present simulation. Instead, COAL as a nonconventional solid is developed and added into the simulation. This is worked out to model the Coal as of availability of the plant and location. This calls for the indigenous simulation of the horizontal feeder gasifier, which is generic and robust. See table 4.9 for a list of the nonconventional properties that are entered for the coal stream.

4.10.3 Simulating the Coal Gasifier

As indicated in figure 4.7, the Coal gasifier is simulated into two different blocks, HORIZONTAL FEEDER and GASIFIER.

The first block, HORIZONTAL FEEDER, is simulated as a Horizontal Equilibrium Reactor. The input to this block is the coal stream and steam. Composition is provided in table 4.9. For this specific process, the products of reaction are the coal constituents in elemental form: C, O_2, H_2 and H_2O from Steam stream. The product yields of this reaction are calculated from the proximate and ultimate analyses and steam. There is no reaction which is taking place in this reactor. Reactor length is taken to be 10 ft and diameter is 9 inch.

The second block, GASIFIER, is simulated as a Gibbs Reactor. A Gibbs reactor is used to model reactions that come to equilibrium by calculating the chemical and phase equilibrium from calculations of minimization of the total Gibbs free energy of the system. The inputs to this block are the decomposed coal and slurry water from horizontal feeder, pressurized oxygen and energy stream. The products of reaction are: CH_4, H_2, CO, CO_2 and unreacted O_2, H_2O.

In addition to simulating the feed components and products, certain reaction conditions must be specified: pressure, temperature and feed conditions. From the design data values, feed coal is in the form of a concentrated water-slurry, operating in any temperature above 980 K. For our base case, this simulation was carried out at 1273 K (1000°C). The reactor is simulated as an adiabatic reactor. The base case gasifier pressure (hence the pressure of the overall process) was selected at 1 bar. Oxygen and steam are at 30 bar pressure.

Table 4.9: Coal Properties used in the present simulation [3]

Proximate Analysis (% weight)	
Moisture	**7**
Ash	**40**
Volatile Matter	**23**
Fixed Carbon	**30**
Ultimate Analysis (% weight)	
Carbon	**75.5**
Hydrogen	**6.4**
Nitrogen	**1.5**
Sulfur	**1.4**
Oxygen	**15.2**

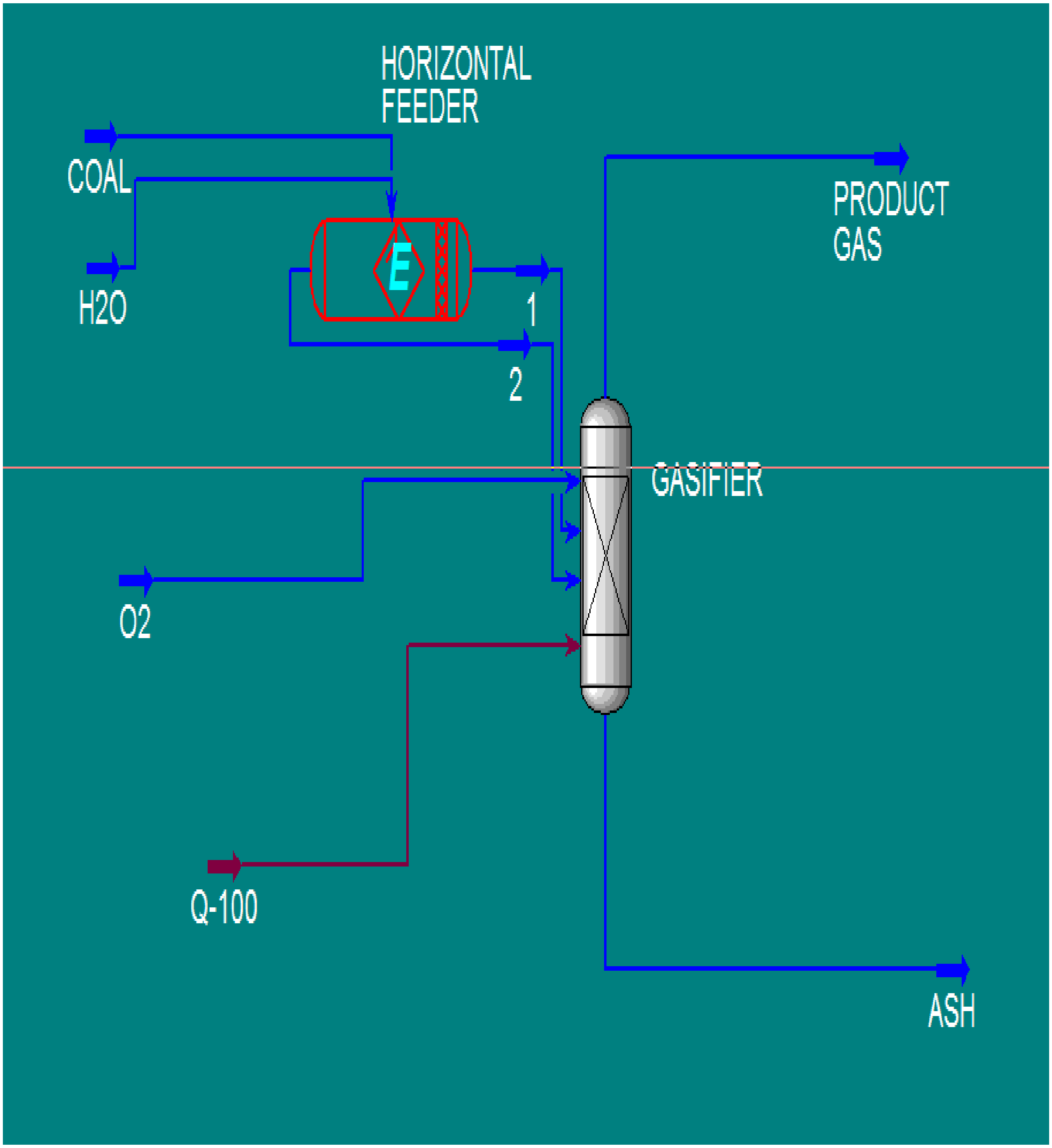
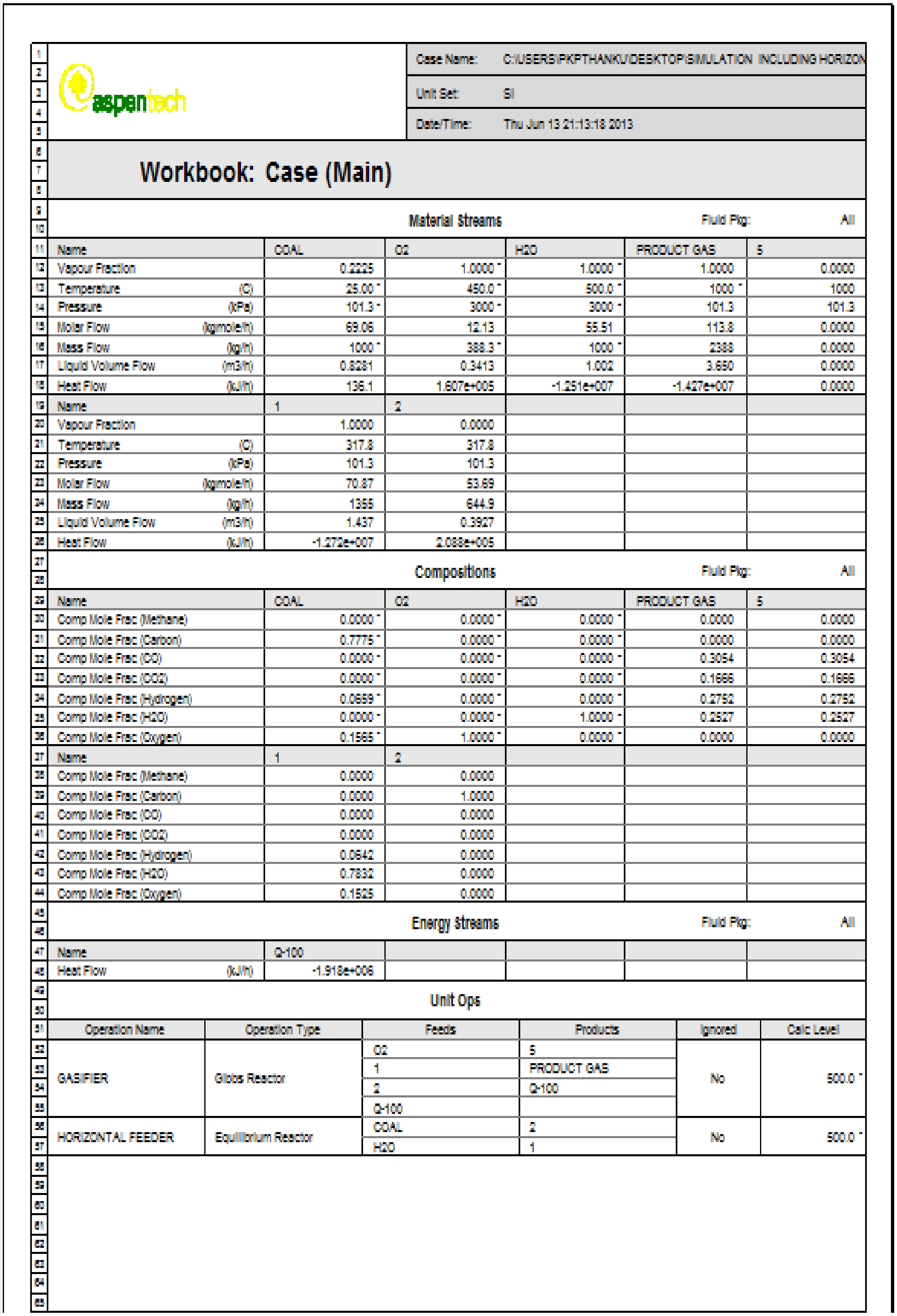


Fig 4.7: Horizontal Feeder Gasifier Simulation Flowsheet

HHV in MJ/kg = 33.86 * C + 144.4 * (H-O/8) + 9.428 * S

HHV= 32.194 MJ/kg

HHV = 13840.926897 BTU/lb



Case Name:	C:\USERS\PKPTHANKU\DESKTOP\SIMULATION INCLUDING HORIZON
Unit Set:	SI
Date/Time:	Thu Jun 13 21:13:18 2013

Workbook: Case (Main)

Material Streams Fluid Pkg: All

Name	COAL	O2	H2O	PRODUCT GAS	5
Vapour Fraction	0.2225	1.0000 *	1.0000 *	1.0000	0.0000
Temperature (C)	25.00 *	450.0 *	500.0 *	1000 *	1000
Pressure (kPa)	101.3 *	3000 *	3000 *	101.3	101.3
Molar Flow (kgmole/h)	69.06	12.13	55.51	113.8	0.0000
Mass Flow (kg/h)	1000 *	388.3 *	1000 *	2388	0.0000
Liquid Volume Flow (m3/h)	0.8281	0.3413	1.002	3.650	0.0000
Heat Flow (kJ/h)	136.1	1.607e+005	-1.251e+007	-1.427e+007	0.0000
Name	**1**	**2**			
Vapour Fraction	1.0000	0.0000			
Temperature (C)	317.8	317.8			
Pressure (kPa)	101.3	101.3			
Molar Flow (kgmole/h)	70.87	53.69			
Mass Flow (kg/h)	1355	644.9			
Liquid Volume Flow (m3/h)	1.437	0.3927			
Heat Flow (kJ/h)	-1.272e+007	2.088e+005			

Compositions Fluid Pkg: All

Name	COAL	O2	H2O	PRODUCT GAS	5
Comp Mole Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (Carbon)	0.7775 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (CO)	0.0000 *	0.0000 *	0.0000 *	0.3054	0.3054
Comp Mole Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	0.1666	0.1666
Comp Mole Frac (Hydrogen)	0.0659 *	0.0000 *	0.0000 *	0.2752	0.2752
Comp Mole Frac (H2O)	0.0000 *	0.0000 *	1.0000 *	0.2527	0.2527
Comp Mole Frac (Oxygen)	0.1565 *	1.0000 *	0.0000 *	0.0000	0.0000
Name	**1**	**2**			
Comp Mole Frac (Methane)	0.0000	0.0000			
Comp Mole Frac (Carbon)	0.0000	1.0000			
Comp Mole Frac (CO)	0.0000	0.0000			
Comp Mole Frac (CO2)	0.0000	0.0000			
Comp Mole Frac (Hydrogen)	0.0642	0.0000			
Comp Mole Frac (H2O)	0.7832	0.0000			
Comp Mole Frac (Oxygen)	0.1525	0.0000			

Energy Streams Fluid Pkg: All

Name	Q-100				
Heat Flow (kJ/h)	-1.918e+006				

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
GASIFIER	Gibbs Reactor	O2 1 2 Q-100	5 PRODUCT GAS Q-100	No	500.0 *
HORIZONTAL FEEDER	Equilibrium Reactor	COAL H2O	2 1	No	500.0 *

Fig. 4.8: Base Case Result Summary

4.11 OPTIMIZATION OF THE PROCESS

The optimization mainly focuses on the production of hydrogen rich synthesis gas along with the CO_2 and H_2O. This can be done by study of variation of product gas with stream variables like gasification temperature, coal mass flow, steam mass flow, O_2 mass flow, etc. Many attempts have been made recently [19-21] to enhance this ratio of H_2/CO. **The achievement of a ratio of 3 is the success of the present study.** See figure 4.18 for more details.

RESULTS AND DISCUSSIONS

4.11.1 Effect of Variation of Gasifier Temperature on Product Gas Composition

Keeping Coal Flow rate =1000 kg/hr. Oxygen Flow rate = 560 kg/hr, Steam Flow rate =500 kg/h. Varying temperature from 600^0C to 1200^0C, mole fractions of outlet gas are calculated and tabulated. From figures 4.12 and 4.13, it is seen that H_2 formation is increased initially and then gets dripped off as the temperature increases. CO and H_2O formation increases as the temperature increases. CO_2 formation also drips off as the temperature increases.

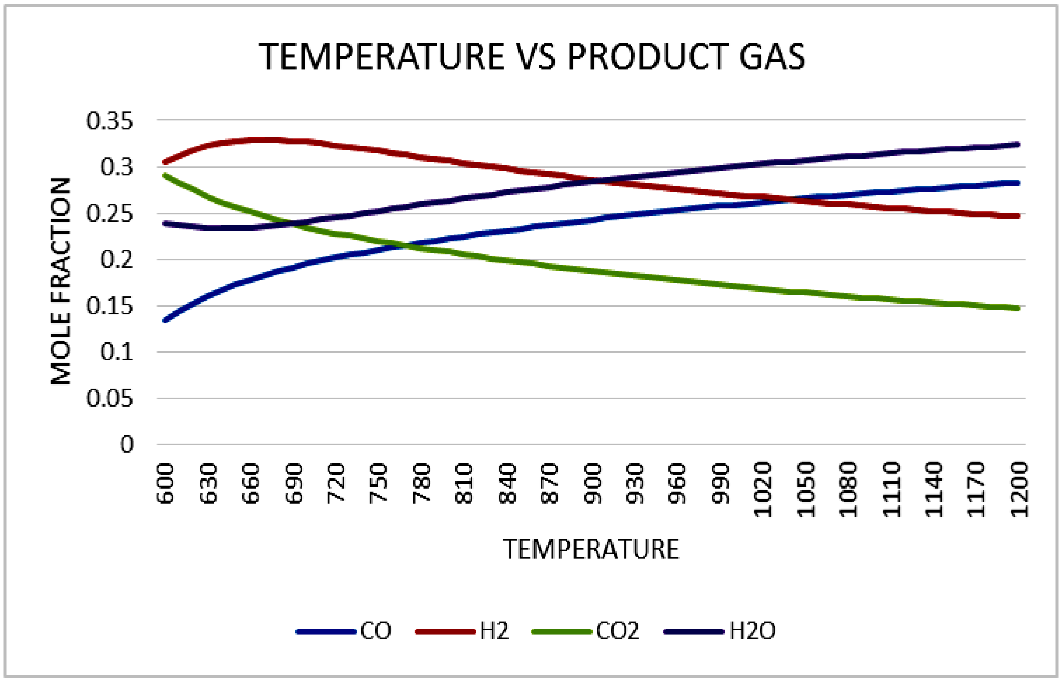


Fig. 4.9: Effect of variation of gasifier temperature on product gas composition

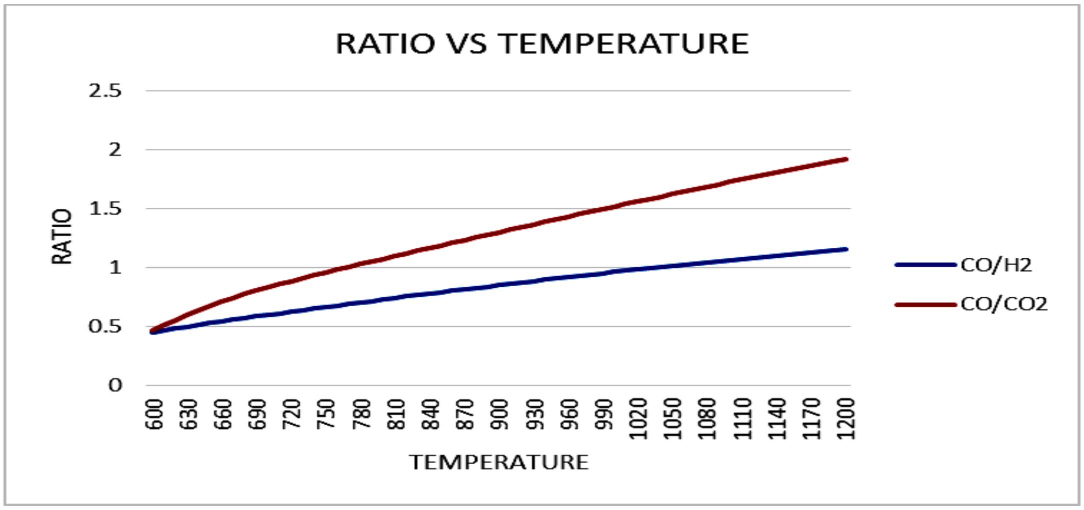


Fig. 4.10: Effect of variation of gasifier temperature on product gas composition ratio

4.11.2 Effect of Variation of Coal Mass Flow on Product Gas Composition

Keeping temperature =1000^{0}C. Oxygen Flow rate = 560 kg/hr, Steam Flow rate =500 kg/h. Varying Coal Flow rate from 500-2000 kg/hr mole fraction of outlet gas are calculated and tabulated.

Table 4.10: Effect of variation of coal mass flow on product gas composition

COAL [kg/h]	Mole Frac CO	Mole Frac H2	Mole Frac CO2	Mole Frac H2O	C0/H2	CO/CO2
500	5.03E-02	0.181154022	0.247406883	0.521110486	0.27745207	0.20315343
600	7.97E-02	0.231061444	0.255757655	0.433198402	0.34500384	0.31168993
700	0.111640428	0.268639586	0.257273191	0.361747369	0.41557698	0.43393728
800	0.144858218	0.296368993	0.253851169	0.303469195	0.48877656	0.57064231
900	0.178474794	0.316251323	0.246981381	0.255712317	0.56434481	0.72262449
1000	0.21185045	0.329893252	0.237793824	0.216353982	0.64217879	0.89089971
1100	0.244559322	0.33857396	0.227118831	0.183710007	0.72232171	1.07679016
1200	0.27634011	0.343304286	0.215550573	0.156453869	0.80494221	1.28201983
1300	0.307049968	0.34487876	0.203505385	0.133545045	0.89031278	1.50880513
1400	0.336626696	0.343919973	0.191270249	0.114167994	0.97879368	1.75995324
1500	0.365060291	0.340915137	0.179040441	9.77E-02	1.07082453	2.03898231
1600	0.392372809	0.33624533	0.166947418	8.36E-02	1.16692419	2.35027779
1700	0.41860472	0.330208422	0.155078862	7.15E-02	1.2676985	2.69930224
1800	0.443806014	0.323036781	0.143492781	6.10E-02	1.37385598	3.09288043
1900	0.468030585	0.314910844	0.132227317	5.20E-02	1.48623204	3.53959071
2000	0.491332826	0.305969435	0.121307529	4.41E-02	1.60582323	4.05030775
1500	0.42327121	0.298973231	9.98E-02	0.177962089	1.41574953	4.24149092
1550	0.435207699	0.302414154	9.53E-02	0.167118577	1.43911154	4.56867488
1600	0.446815303	0.305623467	9.08E-02	0.156776476	1.46197969	4.92173068
1650	0.458106438	0.308618846	8.64E-02	0.146903621	1.4843761	5.30397174
1700	0.469093039	0.311416333	8.20E-02	0.137470501	1.50632125	5.71929343
1750	0.479786562	0.314030514	7.77E-02	0.128449992	1.52783421	6.17230758
1800	0.490197989	0.316474677	7.35E-02	0.119817118	1.54893274	6.66851611
1850	0.500337844	0.318760952	6.94E-02	0.111548845	1.56963343	7.21453746
1900	0.5102162	0.320900424	6.53E-02	0.103623893	1.58995178	7.81840589
1950	0.519842695	0.322903248	6.12E-02	9.60E-02	1.60990234	8.48997229
2000	0.529226549	0.324778735	5.73E-02	8.87E-02	1.62949877	9.24144924

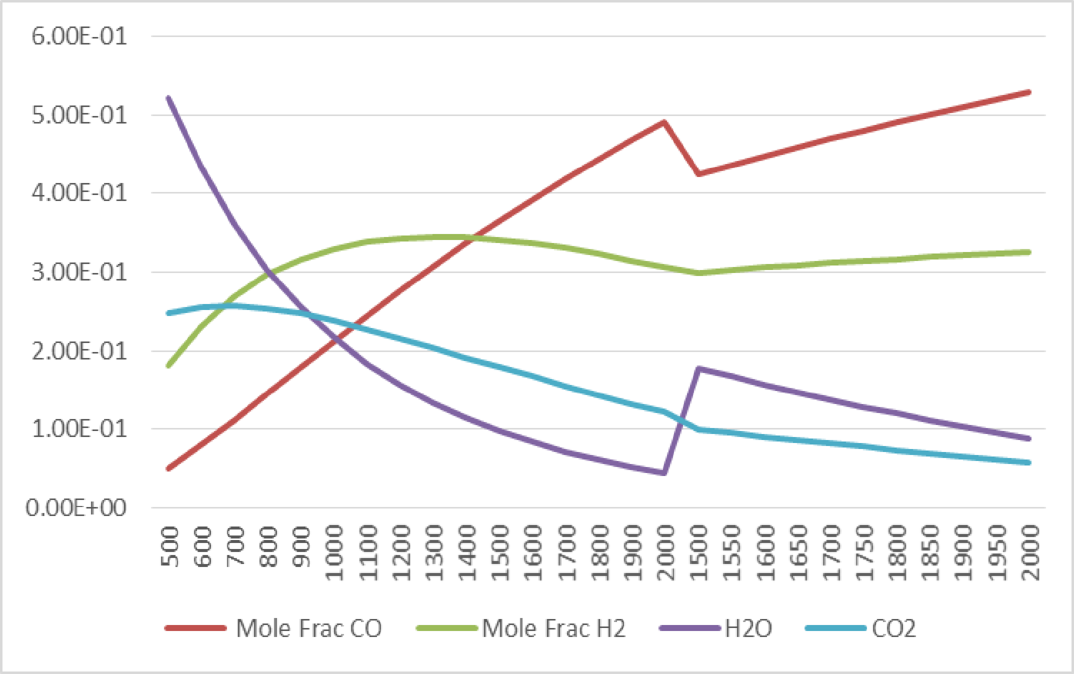


Fig. 4.11: Effect of variation of coal mass flow on product gas composition

Figure 4.14 shows that, Synthesis gas production increases with the coal flow rate. Optimum flow rate for this condition is 1000-1200 kg/hr. At this flow rate, hydrogen production is sufficiently high and CO_2 production is low. Above 1400 kg/hr flow rate, CO production is much more than hydrogen, hence it is not preferred.

4.11.3 Effect of Variation of Steam Mass Flow on Product Gas Composition

Keeping gasification temperature =1000^{0}C. Oxygen Flow rate = 560 kg/hr, Coal Flow rate =1000 kg/h. Varying Coal Flow rate from 500-2000 kg/hr and mole fraction of outlet gas are calculated and tabulated

As the steam rate increases mole fraction of CO decreases and hydrogen increases up to 0.3 from 1400 kg/hr. Later, H_2 reduces. Best steam flow rate can be between 1200 -1400 kg/hr.

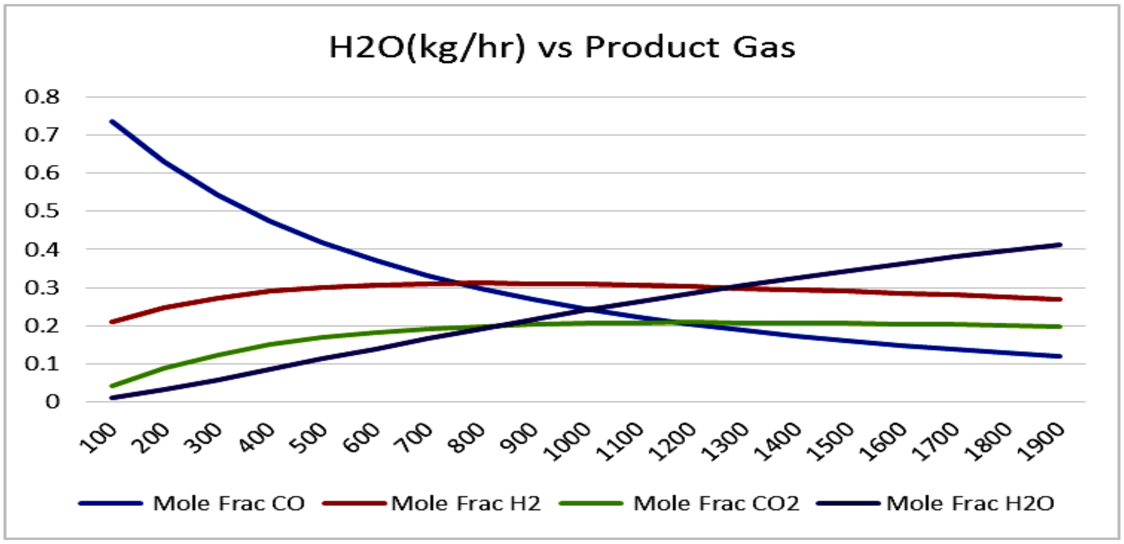


Fig. 4.12: Effect of variation of steam mass flow on product gas composition

Table 4.11: Effect of variation of steam mass flow on product gas composition

H2O [kg/h]	Mole Frac CO	Mole Frac H2	Mole Frac CO2	Mole Frac H2O	C0/H2	CO/CO2
100	0.867393823	9.18E-02	1.22E-03	1.19E-04	9.44803238	712.804111
200	0.735224089	0.208257198	4.14E-02	1.08E-02	3.5303658	17.7572253
300	0.629287496	0.24793023	8.85E-02	3.22E-02	2.53816364	7.10991317
400	0.544353848	0.273469538	0.123528763	5.73E-02	1.99054656	4.40669716
500	0.475348769	0.290303633	0.149239875	8.41E-02	1.63741929	3.18513246
600	0.418563876	0.301072219	0.168052847	0.11159538	1.3902441	2.49066817
700	0.371296412	0.307492602	0.181726726	0.138941009	1.20749706	2.04315799
800	0.331546221	0.310755141	0.191537356	0.165741534	1.06690502	1.7309742
900	0.297809402	0.311707805	0.198418868	0.191734986	0.95541208	1.50091271
1000	0.268938362	0.310965122	0.203063117	0.216772523	0.86485057	1.32440773
1100	0.244045526	0.308978193	0.205988264	0.240778943	0.78984709	1.18475452
1200	0.222435965	0.306081564	0.207586373	0.263726961	0.72672121	1.07153452
1300	0.203559489	0.302525424	0.208156856	0.285620232	0.67286738	0.97791393
1400	0.186976035	0.298498157	0.207930264	0.306482067	0.62638924	0.89922472
1500	0.172330327	0.29414238	0.207085434	0.326347872	0.58587385	0.8321702
1600	0.159333065	0.289566494	0.205761993	0.345260081	0.5502469	0.77435615
1700	0.147746795	0.284853121	0.204069579	0.363264756	0.51867711	0.72400205
1800	0.137375178	0.280065307	0.202094708	0.380409322	0.49051123	0.67975643
1900	0.128054764	0.275251144	0.19990594	0.396741072	0.46522882	0.64057508
2000	0.119648613	0.270447236	0.197557794	0.412306205	0.44241019	0.60563853

4.11.4 Effect of Variation of Oxygen Mass Flow on Product Gas Composition

Keeping gasification temperature =1000^0C. Steam Flow rate = 1100 kg/hr, Coal Flow rate =1000 kg/h. Varying Oxygen Flow rate from 500-2000 kg/hr and mole fraction of outlet gas are calculated and tabulated.

The effect of oxygen flow rate was studied on product gas composition. The composition of H_2 decreases with very small deviation. The composition of CO and H_2O increases with increase in the oxygen rate which means that in the stoichiometric reactor, the reactions of carbon with oxygen, i.e. complete and partial oxidation, takes place. Ideal flow rate of oxygen is between 140-150 kg/hr.

Table 4.12: Effect of variation of oxygen mass flow on product gas composition

MASS FLOW O2	Mole Frac CO	Mole Frac H2	Mole Frac CO2	Mole Frac H2O	CO/H2	CO/CO2
100	0.275804132	0.39354652	0.172889134	0.144131225	0.7008171	1.59526586
150	0.264848249	0.383926438	0.184084298	0.155907462	0.68984113	1.43873351
200	0.253804331	0.373646403	0.195330477	0.168010061	0.67926341	1.29935858
250	0.242698135	0.362761493	0.206606969	0.180429503	0.66902949	1.17468513
300	0.231554035	0.351321007	0.217893823	0.193156335	0.65909533	1.06269205
350	0.220394971	0.339369202	0.229171968	0.206181179	0.64942537	0.96170126
400	0.209242411	0.326945893	0.240423326	0.219494746	0.63999094	0.87030828
450	0.198116304	0.31408695	0.25163091	0.23308787	0.63076898	0.78732896
500	0.18703506	0.300824723	0.262778898	0.24695153	0.62174099	0.71175829
550	0.176015538	0.287188402	0.273852692	0.261076885	0.61289222	0.64273802
600	0.165073047	0.273204326	0.284838945	0.275455304	0.60421096	0.57953117
650	0.154221373	0.258896263	0.295725579	0.290078393	0.59568791	0.52150164
700	0.143472813	0.244285649	0.306501774	0.304938017	0.58731577	0.46809782
750	0.13283822	0.229391806	0.317157948	0.32002633	0.57908877	0.41883932
800	0.122327068	0.214232136	0.327685723	0.335335784	0.57100242	0.37330607
850	0.111947515	0.198822292	0.338077874	0.350859154	0.56305314	0.33112938
900	0.101706482	0.183176336	0.348328278	0.366589549	0.55523811	0.29198457
950	9.16E-02	0.167306874	0.358431851	0.382520422	0.54755505	0.25558477
1000	8.17E-02	0.151225187	0.368384482	0.398645582	0.54000209	0.22167578

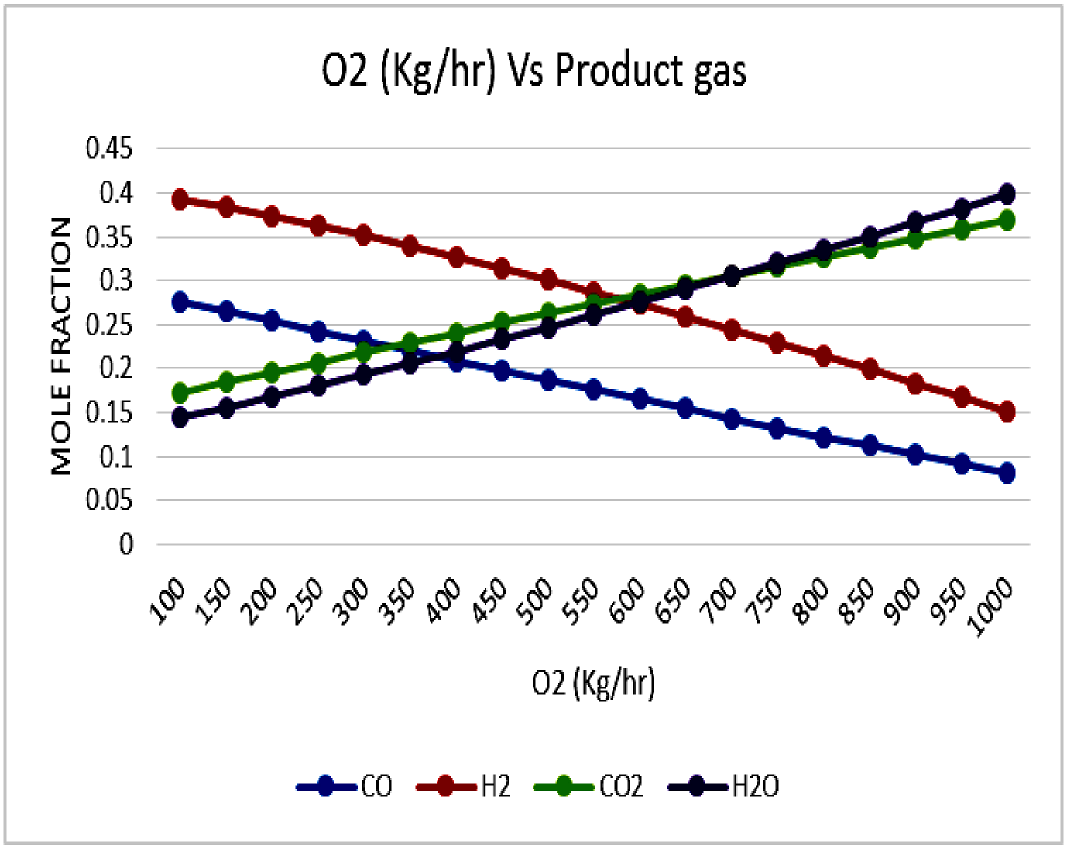


Fig. 4.13: Effect of variation of oxygen mass flow on product gas composition

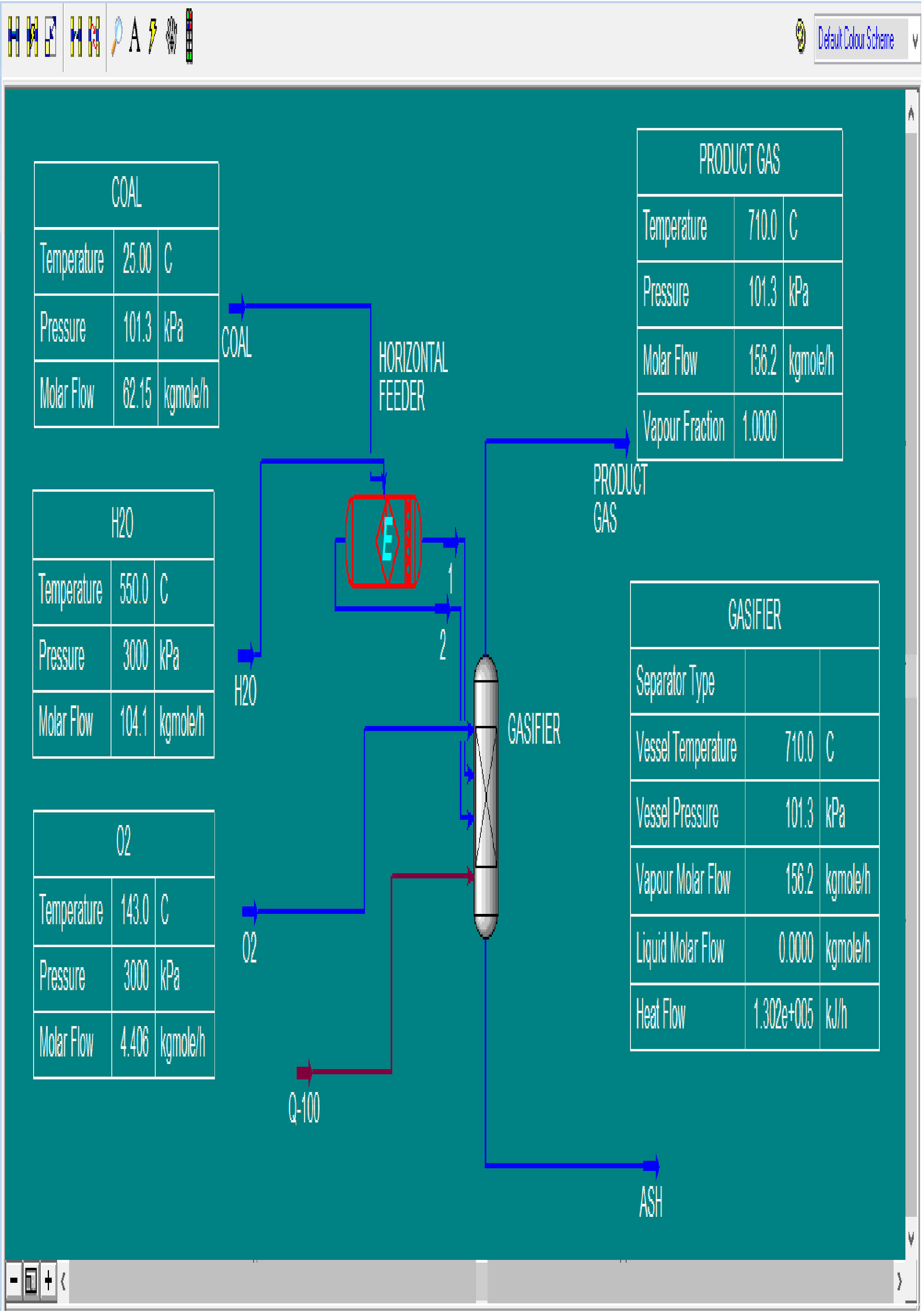
CONCLUSIONS

A process optimization method has been developed and applied to study the coal gasification for the production of synthesis gas. The boundary definition and the identification of main units are basic steps for the process analysis. Thermodynamic databases, parametric models and steady state simulation software are fundamental tools, which are appropriately combined to gain the specific advantages**.**

A simulation study using ASPEN HYSYS was performed considering a coal sample using its proximate and ultimate analysis and the effects of various operating parameters were studied on the product gas composition.

Simulation trials were conducted by varying the steam flow rates thereby changing the steam, coal, oxygen flow rate whereas the temperature and all other parameters were kept constant. The extremely low composition of CO_2 can be attributed to the simplifications used in the simulation. There is a competition between the several gasification reactions to reach completion so it is very difficult to access the product gas composition as it also depends upon the operating parameters. The purpose of gasification dictates the presence or absence of a gasifying agent. From the study of optimization, observations are made for coal at flow rate of 1000kg/hr. The H_2: CO mole ratio of 3.04:1 could be obtained using the optimized scheme.

With the favorable results from the present study of innovative design of horizontal feeder gasifier, we decided to adopt another innovative approach for power production in power plants, especially with recent technological outcomes of IGCCs. We decided to try different combinations of feeds to gas turbines instead of depending on only one fuel type. The details are explained in the upcoming chapter 5.



COAL		
Temperature	25.00	C
Pressure	101.3	kPa
Molar Flow	62.15	kgmole/h

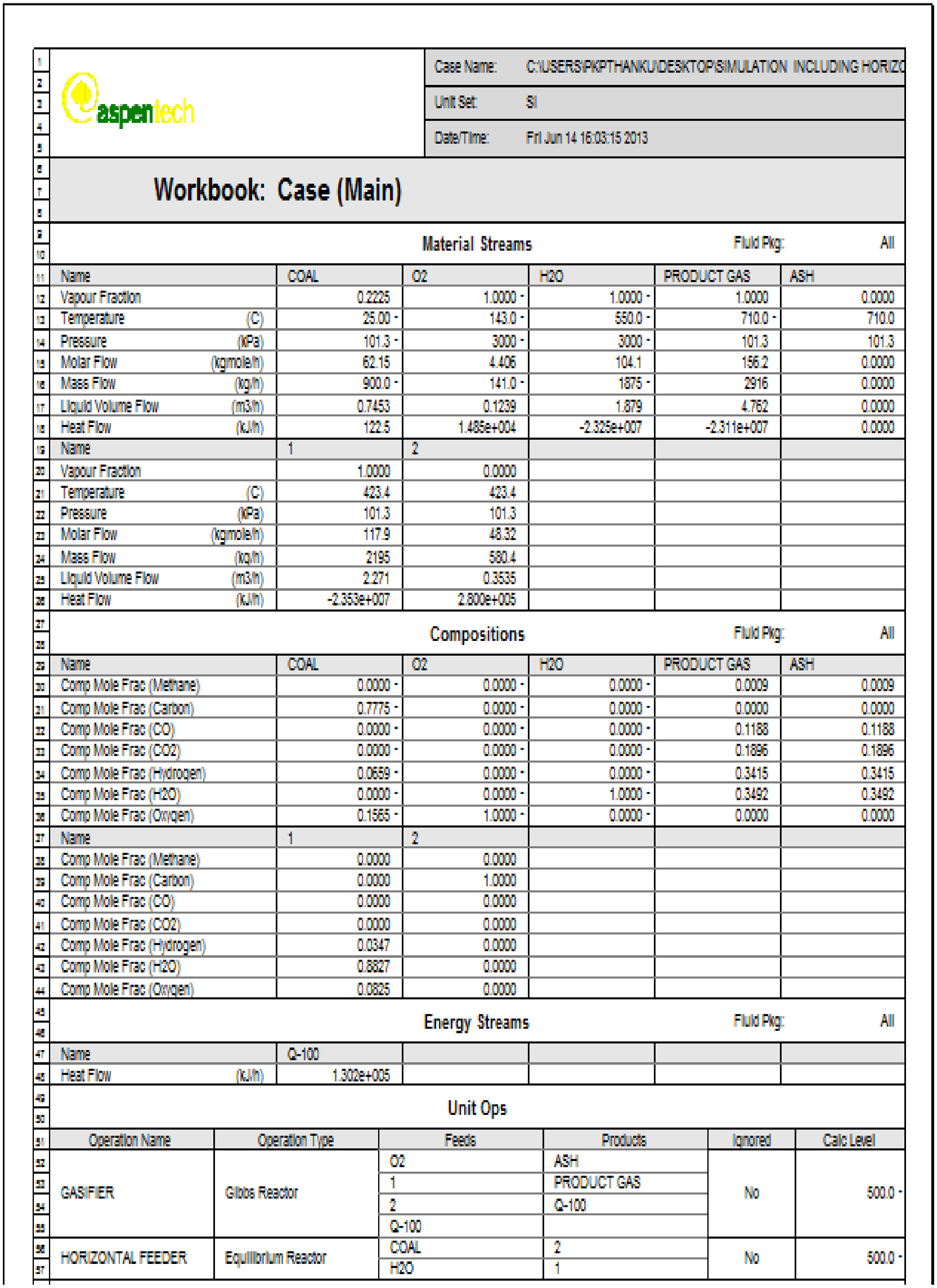
H2O		
Temperature	550.0	C
Pressure	3000	kPa
Molar Flow	104.1	kgmole/h

O2		
Temperature	143.0	C
Pressure	3000	kPa
Molar Flow	4.406	kgmole/h

PRODUCT GAS		
Temperature	710.0	C
Pressure	101.3	kPa
Molar Flow	156.2	kgmole/h
Vapour Fraction	1.0000	

GASIFIER		
Separator Type		
Vessel Temperature	710.0	C
Vessel Pressure	101.3	kPa
Vapour Molar Flow	156.2	kgmole/h
Liquid Molar Flow	0.0000	kgmole/h
Heat Flow	1.302e+005	kJ/h

Fig. 4.14: Optimized Horizontal Feeder Coal Gasifier Simulation Flowsheet



aspentech

Case Name:	C:\USERS\PKPTHANKU\DESKTOP\SIMULATION INCLUDING HORIZ
Unit Set:	SI
Date/Time:	Fri Jun 14 16:03:15 2013

Workbook: Case (Main)

Material Streams Fluid Pkg: All

Name		COAL	O2	H2O	PRODUCT GAS	ASH
Vapour Fraction		0.2225	1.0000 *	1.0000 *	1.0000	0.0000
Temperature	(C)	25.00 *	143.0 *	550.0 *	710.0 *	710.0
Pressure	(kPa)	101.3 *	3000 *	3000 *	101.3	101.3
Molar Flow	(kgmole/h)	62.15	4.406	104.1	156.2	0.0000
Mass Flow	(kg/h)	900.0 *	141.0 *	1875 *	2916	0.0000
Liquid Volume Flow	(m3/h)	0.7453	0.1239	1.879	4.762	0.0000
Heat Flow	(kJ/h)	122.5	1.485e+004	-2.325e+007	-2.311e+007	0.0000
Name		1	2			
Vapour Fraction		1.0000	0.0000			
Temperature	(C)	423.4	423.4			
Pressure	(kPa)	101.3	101.3			
Molar Flow	(kgmole/h)	117.9	48.32			
Mass Flow	(kg/h)	2195	580.4			
Liquid Volume Flow	(m3/h)	2.271	0.3535			
Heat Flow	(kJ/h)	-2.353e+007	2.800e+005			

Compositions Fluid Pkg: All

Name	COAL	O2	H2O	PRODUCT GAS	ASH
Comp Mole Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0009	0.0009
Comp Mole Frac (Carbon)	0.7775 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (CO)	0.0000 *	0.0000 *	0.0000 *	0.1188	0.1188
Comp Mole Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	0.1896	0.1896
Comp Mole Frac (Hydrogen)	0.0659 *	0.0000 *	0.0000 *	0.3415	0.3415
Comp Mole Frac (H2O)	0.0000 *	0.0000 *	1.0000 *	0.3492	0.3492
Comp Mole Frac (Oxygen)	0.1565 *	1.0000 *	0.0000 *	0.0000	0.0000
Name	1	2			
Comp Mole Frac (Methane)	0.0000	0.0000			
Comp Mole Frac (Carbon)	0.0000	1.0000			
Comp Mole Frac (CO)	0.0000	0.0000			
Comp Mole Frac (CO2)	0.0000	0.0000			
Comp Mole Frac (Hydrogen)	0.0347	0.0000			
Comp Mole Frac (H2O)	0.8827	0.0000			
Comp Mole Frac (Oxygen)	0.0825	0.0000			

Energy Streams Fluid Pkg: All

Name		Q-100				
Heat Flow	(kJ/h)	1.302e+005				

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
GASIFIER	Gibbs Reactor	O2 1 2 Q-100	ASH PRODUCT GAS Q-100	No	500.0 *
HORIZONTAL FEEDER	Equilibrium Reactor	COAL H2O	2 1	No	500.0 *

Fig. 4.15: Optimized Horizontal Feeder Coal Gasifier Simulation Flowsheet Base Case Result Summary

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CHAPTER -5

SIMULATION AND OPTIMIZATION OF COMBINED FEED IGCC POWER PLANT

This chapter elaborates another innovative approach to resolve the difficulty of power plants arising due to scarcity of one type of fuel and reduce their dependency on specific fuels. Many power stations are not producing power to their capacity as fuel like good quality coal is not available as of requirement. Because of the energy that it is able to provide by virtue of its calorific value, over dependency on any fuel like natural gas or naphtha is inevitable. As a result, depletion of a particular fuel becomes a consequence. Therefore, steps are taken these days to check for the viability of other fuels that may/can be used in combination with one another in order to overcome this limitation. The purpose of this study is to explore the idea expressed above. In this sense, we have focused on power generation from an Integrated Gas Combined Cycle (IGCC) plant by allowing the syngas that comes out of the gasifier to blend itself in various configurations. The study reveals important results such as the fuel gas temperature and pressure of feed to the gas turbine are in direct proportion with the power produced in gas turbine. As fuel gas temperature and stream pressure increases, the power produced increases. The optimum value of the temperature of fuel gas is taken as 900-1500 ^{0}C. The overall power generated is calculated for different combinations of feed pressures. The objective of this study identifies the importance of keeping the H_2/CO ratio intact. This is facilitated by the increase in calorific value through the combination of various fuels. In the process, we have considered blending of syngas and natural gas as a case study that could possibly find its solution rooted in this very thesis. The numerous simulations and pragmatic case studies will provide sound information on the viability and feasibility in operation of such an approach which is not practiced anywhere in the world and is in the research and development stage.

Keywords: scarcity of fuels, fuel depletion, gasification efficiency, IGCCs, combined feed power plants, optimization, natural gas

5.1 INTRODUCTION

Though this topic potentially deals with the effects that a combined feed cycle will have on power generation, we shall start by divulging the context of the chapter through the significant appreciations of the fuels required to instigate the process at hand. We shall proceed with the basic types of fuels required by many industries, power plants in particular, across the globe and subsequently delve into the various aspects, such as the availability, transportation costs and suitability to a process based on immediate requirements. Some basic fuels considered in this study are:

a) Coal
b) Biomass
c) Naphtha and Natural gas

These fuel types and their availability are briefly explained below.

5.1.1 Coal

Coal supplies 80% of the worlds energy demand and forms the bulk of the utilization of fossil sources. The fact that it is abundant is down to it being the most abundant and relatively cheap form of fuel.

5.1.1.1 Importance and Availability

Today, coal is often the fuel of choice for electricity generation and perhaps will be the major source for extensive synthetic liquid productions in the future in many parts of the world. Its low cost and wide availability make it especially attractive in major developing economies for meeting their pressing energy needs. It has been estimated that there are over 984 billion tonnes of proven coal reserve worldwide [1]. This means that there is enough coal to last us over 190 years.

5.1.1.2 Power generation from Coal

Steam coal, also known as thermal coal, is used in power stations to generate electricity. The earliest conventional coal-fired power stations used lump coal which was burnt in boilers to raise steam. Nowadays, the coal is first milled to a fine powder, which increases the surface area and allows it to burn more quickly. In these pulverized coal combustion (PCC) [2] systems, the powdered coal is blown into the combustion chamber of a boiler where it is burnt at high temperature. Coal currently supplies 39% of the world's electricity. In many countries this role is much higher. The availability of low-cost supplies of coal in both developed and developing countries has been vital to achieving high rates of electrification [3].

5.1.2 Biomass

Biomass is not a well defined feedstock. In fact it can be merely described as some form of organic matter that has found its very rudimentary origins in the common process of photosynthesis and therefore this attributes to its non-homogeneity [4].

Researchers [5, 6] reported that annually, photosynthesis stores 5 – 8 times more energy in biomass than man currently consumes from all sources. It is also stated that biomass is currently the fourth largest energy source in the world, making it in principle the main energy source of the future. Several scenarios for the future predict a strong increase in the use of bio-fuels between 2025 and 2050.

5.1.2.1 Biomass availability

Main sources of biomass energy are trees, crops and animal waste. Until the middle of 19th century, biomass dominated the global energy supply with a seventy percent share [7].

5.1.2.1 Biomass for Electricity Generation

The future of modern biomass power programme rests on its competitive ability vis-à-vis other centralized electricity generation technologies. Policies for realizing biomass electric power potential through modern technologies under competitive dynamics have a recent origin in India. The cost of electricity generation from these plants is anticipated to be quite competitive being around ₹ 1.8 per kWh [8]. Coal power plants are built with large scale technology, with a standard size of 500 MW. Scale of grid based biomass plants vary from a 1 MW to 50 MW. Recent work shows that, successful attempts are made to enhance this power generation capacity to odd 100 MW [9-11].

5.1.3 Naphtha and Natural Gas

Naphtha and natural gas as feedstock are considered as building blocks by the entire petrochemical industry. As feedstock, Naphtha and natural gas are transformed into various industrial and consumer goods. On the one hand, the cost of Naphtha fluctuates as a function of international oil prices and being a major feedstock, it is expensive. In India, in the year 1999, it was costing around ₹ 12040.00 per MT where as it is ₹ 65208.00 per MT in August 2014 [12]. On the other hand, natural gas is much cheaper than Naphtha which costs US$ 4.2 per million BTU (MMBTU) in August 2014 and its price does not vary as much as of Naphtha. The recent price rise demand by natural gas exploring companies, which was due by April 2014, is halted till September 2014 by the new Government of India. The supply of natural gas is controlled by the Oil and Natural Gas Corporation (ONGC) and the Gas Authority of India Ltd. (GAIL) along with Reliance Industries Limited (RIL), having large reservoir estimates in its Krishna-Godawari (KG-D6) block obtained under New Exploration Licensing Policy (NELP-I). Cairn Energy and BP are other major explorers in India.

As feedstock, natural gas and Naphtha are used to produce town gas. By using natural gas in addition to Naphtha, the cost of production of town gas gets reduced by 10%. It also reduces the dependence on any one feedstock. Natural gas as a feedstock is even more beneficial as it emits very low levels of toxic and harmful pollutants such as nitrogen oxides, carbon dioxide, and sulfur oxides. It is much more environment-friendly than Naphtha. Natural gas and Naphtha as feedstock form important components for the formation of nitrogen based fertilizers such as urea. The subsidiaries on feedstock such as Naphtha and natural gas have been removed as a direct aftermath of de-regulations in the hydrocarbons industry. This has led to an increase in the cost of production of nitrogenous fertilizers. Further, natural gas and Naphtha are feedstock for the power supply sector and this also increases the cost of both the items. As the unhindered and regular supply of Naphtha and natural gas as feedstock are quite critical, many companies maintain both the natural gas and Naphtha gas lines. This shows the importance of naphtha and natural gas as a feedstock.

Naphtha and natural gas as feedstock are important for they are the basic chemicals for the formation of many products. So efforts must be taken by the government of India and the petrochemical industry that the supply of natural gas and Naphtha is well maintained.

5.1.3.1 Shift from Naphtha to Natural Gas

India's consumption of natural gas has taken due to a 50% increase in domestic production in recent year. While impediments to supply growth remain, Indian consumption will continue to grow and reach 85 billion cubic meters in the next five years. As natural gas use grows and displaces other fuel, it will reduce some 100,000 bbl/d, or about one-third of the country's naphtha demand [13].

5.1.3.2 Naphtha and Natural Gas for Power Generation

The country's largest power generation utility, NTPC Ltd, has generated more power in its gas-based power plants by increasing the use of naphtha, which is cheaper, in place of liquefied natural gas (LNG), as global demand and prices slide amid the economic slowdown. As a result, a plant running on naphtha needs annual overhauling compared with those using gas that need to be overhauled every five years [14].

5.2 GASIFICATION

Throughout the discussion of the future prospects of certain types of fuels in the previous section, the one thing that stands out is its inferred role in the generation of power. Now there have been significantly many developments in that particular sector over the years, but from the aspect of 'clean power' nothing quite suffices as much as would the concept of gasification. Gasification has been introduced for the sake of generation of clean power as the pollutants from the other diversified categories would entail plenty of emissions that prove to be not only harmful to human health but also have devastating effects on the environment in the long run.

The above discussion intends for production of clean energy. The objective of the topic at present is far from that of whether the energy being produced is clean or not, but energy should be produced and supplied to the world. Moreover, it comprises of the process of gasification and how its application extends to the innovative idea of the combined feed power plants.

During discussions in earlier chapters, gasification has been explained in details. Hence, discussion on gasification, various types of gasifiers, their advantages and disadvantages is not carried out here.

5.3 COMBINED FEED

The prospects of the combined feed turbine implementation in the IGCC through additions of various fuel sources to the syngas as soon as it emanates from the gasifier has the capacity to improve the overall quality of the gas, in terms of attainment of a better H_2/CO ratio. These additions of fuels to the syngas are garnering popularity throughout the world, though no implementations have been carried out yet. And while, it may prove to be a process with a slightly higher capital than that required to set up the IGCC plant, the results will be beneficial not only to the power plants drawing their source of power from such an advancement, but also to any other form of device that requires a better performance in terms of requiring more power. The fact here is the manipulation of the CO/H_2 facilitating the enhancement of power through increased calorific value in the ratio of 1:3 or 1:4.

5.3.1 Present Scenario

Over dependency on the energy that a fuel is able to provide by virtue of its calorific value is inevitable. Depletion of that particular fuel becomes a consequence as a result. Therefore, steps are taken these days to check for the viability of other fuels that may/can be used in combination with one another in order to overcome this limitation. Some of these steps involve blending of ethanol with petrol for running vehicles while others include the harnessing of renewable sources of energy and CNG options.

5.3.2 Objective of the present study

The purpose of the present study is meant to serve moves beyond the ideas mentioned in the immediate preceding section. We shall focus upon power generation from an IGCC plant by allowing the syngas that comes out of the gasifier to blend itself in the following configurations:

a) Syngas only from coal
b) Syngas blended with natural gas
c) Syngas blended with biomass
d) Syngas blended with naphtha

These combinations and their effects on power plants are analyzed by developing simulation cases in Aspen HYSYS®. The comparison is made at the end demonstrating better choices on technical ground. Off course, availability of the fuel supply of preferred category is vital. The outcome of the study is quite encouraging, which helps in reducing power supply difficulties. Also, if practiced, this innovative approach can help in supplying quality power along with reducing wear and tear of electrical instruments.

Table 5.1 shows various feedstocks which can be used for power generation in combination mode.

5.3.3 Opportunity for the study

Many power plants are put on hold due to the unavailability of natural gas. Even more, natural gas is not being provided because of geo-political reasons. The idea to model and develope the plant is for using coal plant and a gas plant to address the requirement of power in the neighboring areas and beyond those regions as well. This would eventually serve to reduce any power cuts occurring due to shortage. However, the downside to this is that natural gas will have to be supplied in significant amounts to run the gas power plants.

Table 5.1: Different feedstocks available for gasification

Coal

- **anthracite**
- **butiminous**
- **sub-butimunous**
- **lignite**

Coke

- **petroleum coke**

Refinery residues

- **organic**
- **inorganic**

Liquid feedstocks

- **orimulsions**
- **oil sands residue**
- **liquid organic residue**
- **coal tar**
- **spent lubricating oil**

Natural gas

Gaseous feeedstocks

- **refinery gas**
- **coke-oven gas**
- **refinery off gas**

Biomass

Wastes

- **solid waste**
- **liquid organic chemical waste**

5.3.4 Possible resolution rendered

One way to overcome any impediment and achieve target of generating desired capacity of power is to combine the available or procurable amounts of natural gas and supply it to the gas turbines in combination with the syngas from coal/biomass gasification, which will enhance the output of power for electricity generation.

This resolution has also warranted for our study to come up with the idea of not just combining natural gas and syngas but also try the other combinations mentioned earlier in section 5.3.2.

Before proceeding to the simulation of the combined feed power plants, working of the combined cycles (CC) plants along with present scenario and their applications in India are discussed below.

5.4 COMBINED CYCLES

Combined cycle plants burn gas or liquid fuels to generate electricity. When natural gas is the fuel, the process is known as Natural Gas Combined Cycle (NGCC). When syngas or syngas-derived gas is the fuel, the process is known as Integrated Gasification Combined Cycle (IGCC). Liquid fuels are generally much more expensive than gaseous fuels, so liquid fueled combined cycle plants are generally limited to locations where gaseous fuels are unavailable.

Coal to liquids and coal to chemicals plants typically consume large quantities of electric power, especially for the air separation unit (ASU). These plants often generate power for internal consumption using a combined cycle plant. The fuel for these plants is either syngas, or a byproduct fuel gas such as the low molecular weight hydrocarbons produced by Fischer-Tropsch synthesis. A combined cycle plant is shown in figure 5.1.

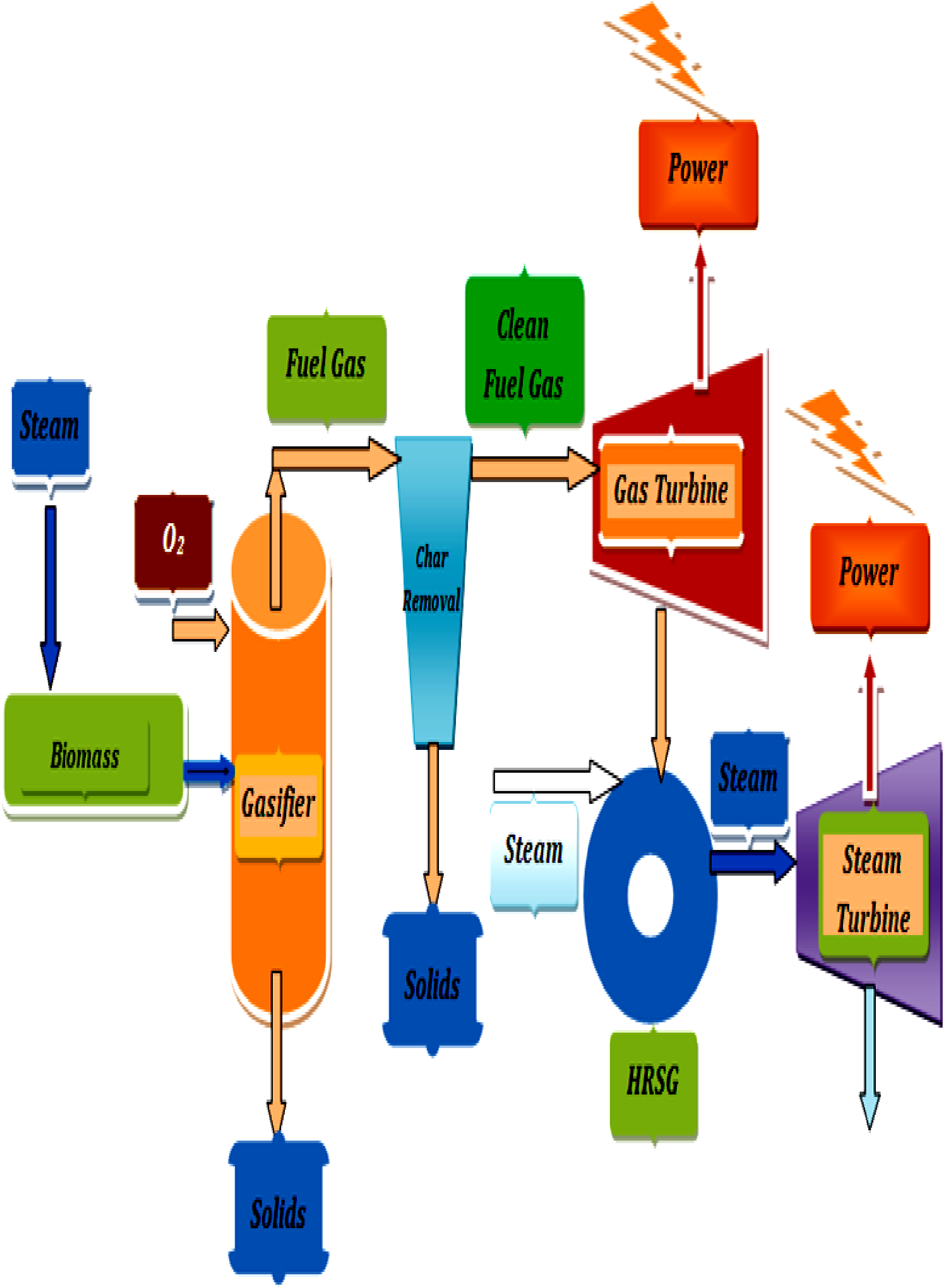


Fig. 5.1: Schematic Representation of Combined Cycle Power Plant [15]

5.4.1 Components for the Combined Cycle

Compressors, combustor and turbines are the major components of a combined cycle. They are explained in details below [15, 16].

5.4.1.1 Compressors

Compressors used in large industrial applications such as power generation are axial flow compressors. In axial flow compressors the fluid enters and leaves in the axial direction.

5.4.1.2 Combustor

The combustor, sometimes referred to as the burner, provides the heat input to the gas turbine cycle. The combustion process is a steady-state flow process in which a hydrocarbon rich fuel is burned with the compressed air to achieve a desired combustor firing temperature.

5.4.1.3 Turbines

In the turbine being of axial-flow type, the flow like in its counterpart, the axial flow compressor, enters and leaves in the axial direction. Similar to the compressor, the turbine consists of a number of stages, each stage consisting of a row of nozzle (stator) blades followed by a row of rotor blades [17].

5.5 TYPES OF COMBINED CYCLES

There are two types of Combined Cycles:

5.5.1 Natural Gas Combined Cycle (NGCC)
5.5.2 Integrated Gasification Combined Cycle (IGCC)

5.5.1 Natural Gas Combined Cycle

Combined cycle can be defined as a combination of two thermal cycles in one plant. This combination of cycle helps in increasing the efficiency of the plant. Thermal cycles with same or with different working media can be combined. The combination used is of gas topping cycle and water/steam bottoming cycle.

Figure 5.2 is a simplified diagram showing the process where the exhaust heat of a simple gas turbine is used to generate steam that will be expanded in a steam turbine [18].

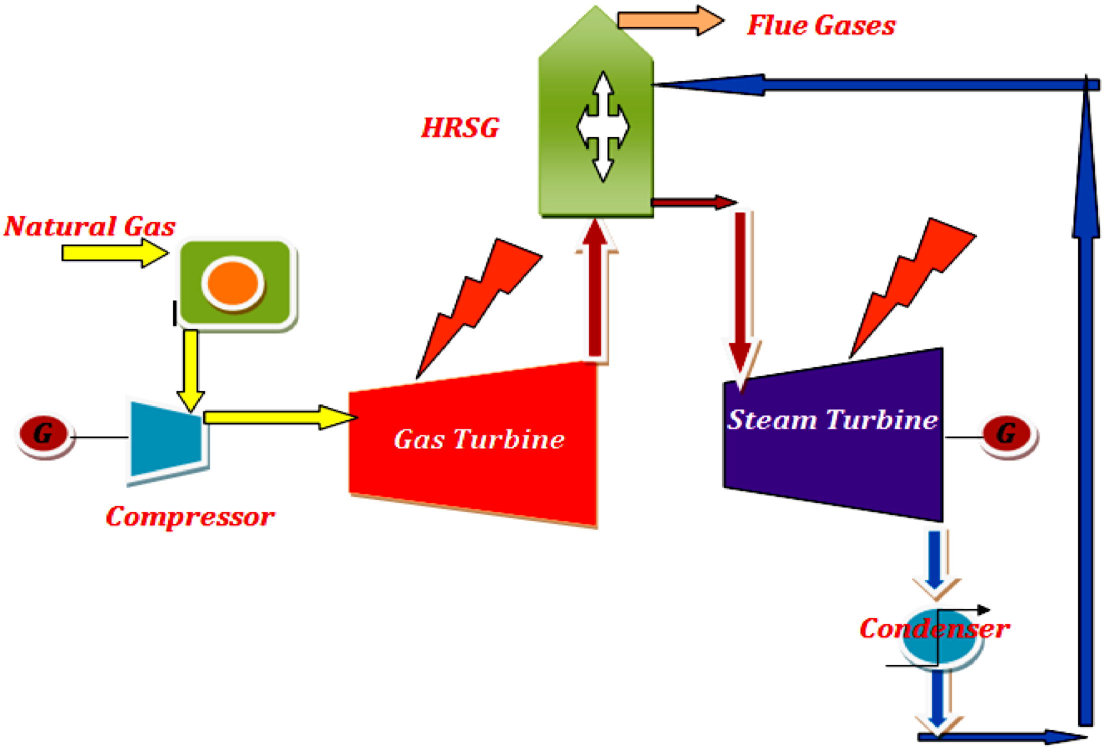


Fig. 5.2: Simplified diagram of NGCC power plant

The gas turbine is one of the most efficient one for the conversion of gas fuels to mechanical power or electricity. The use of distillate liquid fuels, usually diesel, is also common as alternate fuels. The basic principle of the Combined Cycle is simple: burning gas in a gas turbine (GT) produces power, which can be converted to electric power by a coupled generator, along with fairly hot exhaust gases. Routing these gases through a water-cooled heat exchanger produces steam, which can be turned into electric power with a coupled steam turbine and generator.

5.5.2 Integrated Gasification Combined Cycle [15]

An alternative to achieving efficiency improvements in conventional pulverized coal-fired power stations is through the use of gasification technology. IGCC plants use a gasifier to convert coal (or other carbon-based materials) to syngas, which drives a combined cycle turbine.

5.5.2.1 Working principle

The working of an IGCC plant is roughly similar to that of NGCC as described earlier, with the major difference being use of gasification technology to produce syngas. A gasifier converts carbon based material to syngas which can be used with a combined cycle of gas turbine and steam cycle.

5.5.2.2 Feedstock Preparation

The non-integrated ASU separates air cryogenically into its main components, nitrogen and oxygen (95% purity). The coal pre-handling unit consists of a wet rod mill in which the coal feed, medium bituminous coal is crushed and mixed with recycled water, fines and ground into a viscous slurry.

5.5.2.3 The Gasifier

In the gasifier process feed coal/water slurry is mixed with the oxygen. The water in the slurry acts as a temperature moderator and as a hydrogen source in the gasification process.

5.5.2.4 Syngas Cooling and Cleaning

The raw syngas leaving the reactor is first cooled in a radiant syngas cooler producing high pressure steam and then further cooled in two parallel fire tube convective syngas coolers where more high pressure steam is generated.

5.5.2.5 The gas turbine

The air which is purified then compressed and mixed with the clean syngas that has been preheated, and ignited, which causes it to expand. The pressure created from the expansion spins the turbine blades, which are attached to a shaft and a generator, creating electricity.

Heat Recovery Steam Generator

In Heat Recovery Steam Generator highly purified water flows in tubes and the hot gases passes a around that and thus producing steam .The steam then rotates the steam turbine and coupled generator to produce electricity. The hot gases leave the HRSG at around 40 ^{o}C and are discharged into the atmosphere.

5.5.2.6 Efficiency

The efficiency of gasification is at best about 80%, which, assuming 60% for the CC implies that the overall efficiency of an IGCC will not be much higher than 80

× 60/100 = 48%. By adding a ‘shift’ reaction, additional hydrogen can be produced and the CO can be converted to CO_2 which can then be captured and stored. IGCC efficiencies typically reach the mid-40s, although plant designs offering more than 50% efficiencies are achievable [18, 19].

5.5.2.7 Fuels

Syngas can be produced by gasification of coal, petroleum coke, refinery residues, liquid organic residue, biomass, and other carbon based material. The selection of the base fuel will depend upon the quality of syngas produced. Mainly coal serves as the fuel.

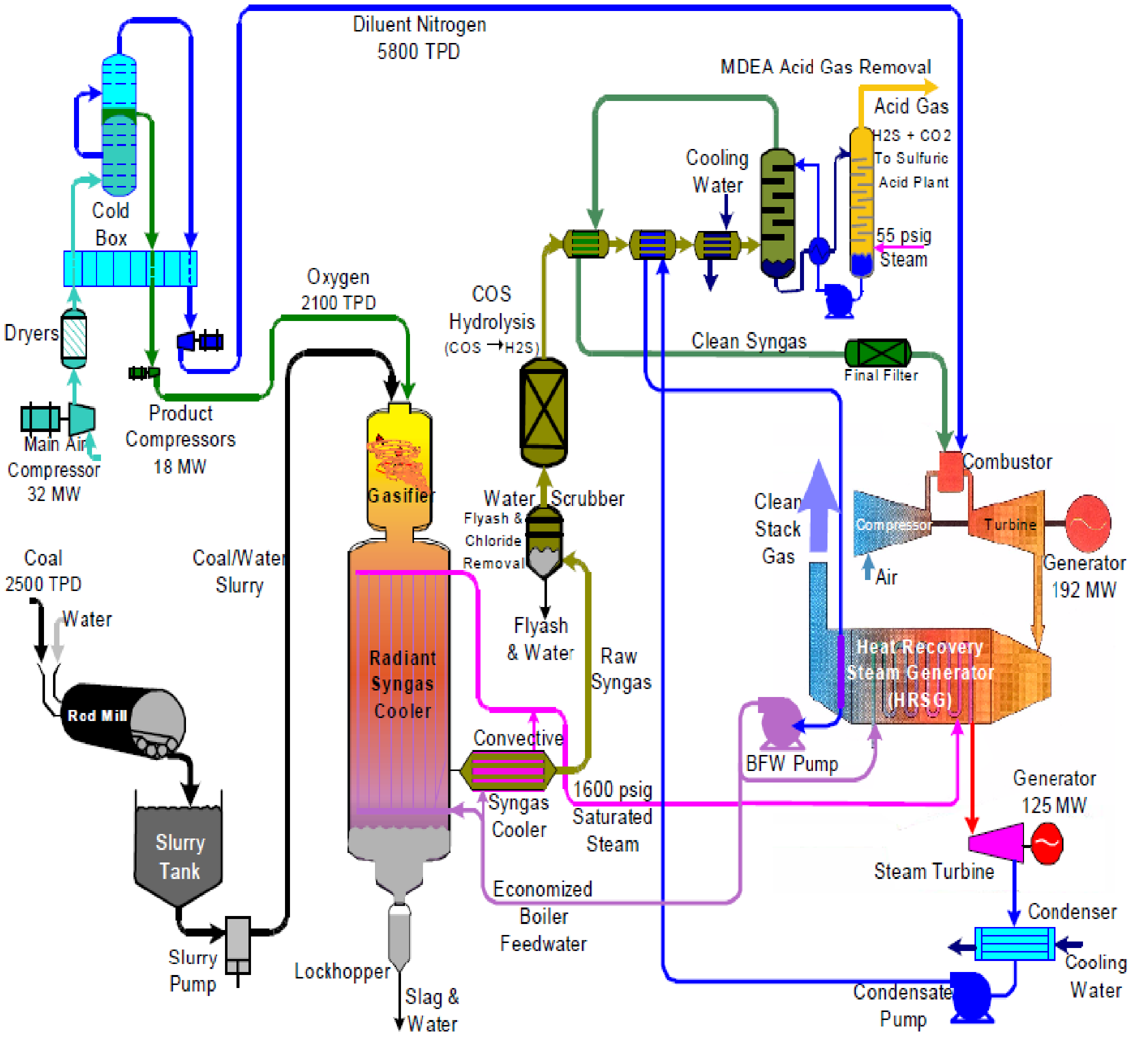


Fig. 5.3: Working of a generalized IGCC power plant [18]

5.6 SIMULATION OF COAL GASIFICATION AND COMBINED FEED IGCC POWER PLANTS

5.6.1 Thermodynamic Study

The gasification process takes place at temperatures in the range 800°C to 1500°C. Over the whole temperature range described above, the reaction rates are sufficiently high that moving on the basis of the thermodynamic equilibrium of the main gaseous components and carbon give results that are close enough to reality that they form the basis of most commercial reactor designs. Detailed thermodynamic study has been carried out in this thesis in chapters 3 and 4 for the various types of gasifiers. The same calculations are used for developing thermodynamic model of gasifier, material and energy balance. As this is already discussed, calculations are not presented here.

Different Combinations considered as Feed for Turbine in Power Plant:

a) Syngas from Coal Gasification.
b) Syngas from Coal and Biomass Gasification.
c) Combined feed from Coal gasification and Naphtha.
d) Combined feed from Coal gasification and Natural gas.

Sections 5.6.2 through 5.6.5 will detail on development of simulation cases for selected systems as mentioned above. The simulation cases flowsheets along with some data results from simulation are provided in various figures below. In these sections, development of combined feed simulations are described in details whereas in sections 5.7 and 5.8, the various optimization methodology and cases for analyzing effects of various key parameters are discussed and results are presented.

5.6.2 Coal

Coal gasification process followed by sending the syngas produced to the power plant is one of the most studied processes. Coal is fed to the gasifier along with steam and oxygen and the gasification process results in generation of combination of gases (CO, H_2, CO_2, H_2O). The combination of (H_2 and CO) is called synthetic gas (syngas). Greater the H_2: CO ratio, greater is the calorific value of fuel gas.

5.6.2.1 Simulation assumptions

- Basis: 1000 kg per hr of coal feed
- All the feed streams are fed at 1000 kg/hr

5.6.2.2 Composition

Table 5.2: Coal properties used in the present simulation [2]

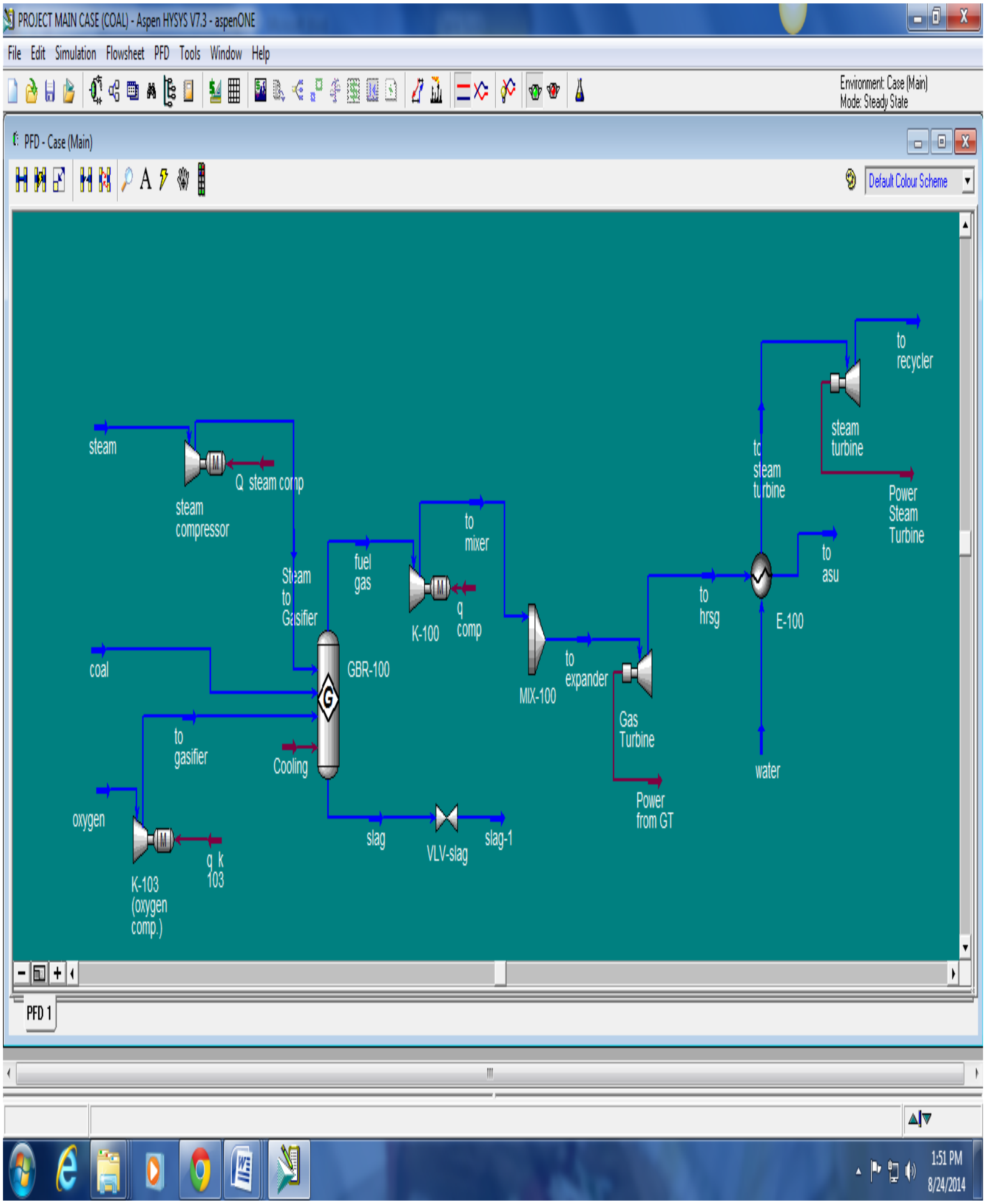
Proximate Analysis (% weight)	
Moisture	7
Ash	40
Volatile Matter	23
Fixed Carbon	30
Ultimate Analysis (% weight)	
Carbon	75.5
Hydrogen	6.4
Nitrogen	1.5
Sulfur	1.4
Oxygen	15.2

5.6.2.3 Steps in developing simulation in Aspen HYSYS®

i. Selection of feed streams
ii. Coal , steam, oxygen are added as feed streams
iii. All feed mass flow rates are 1000 kg/hr, at normal temperature and pressure
iv. Feed is compressed to 7000 kPa using compressor
v. Gibbs reactor is selected which acts as the gasifier
vi. Gas produced at high temperature from gasifier is compressed further to 9000 kPa and sent to gas turbine in power plant.
vii. Power plant is an integrated gasification combined cycle
viii. This consists of gas turbine and followed by heat recovery steam generator and additional steam turbine.
ix. Power production is calculated

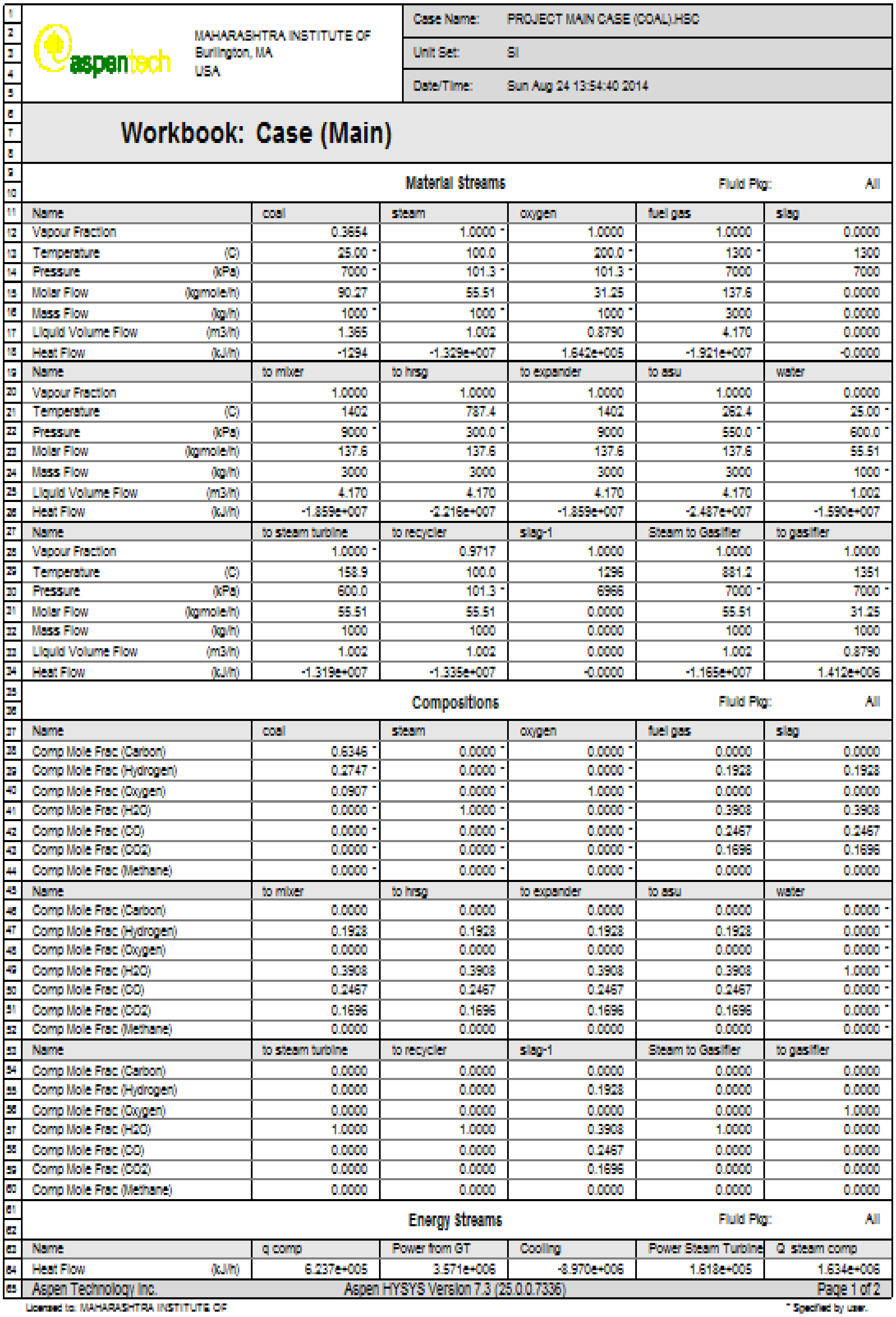
5.6.2.4 Simulation for base case design

Using simulation steps as discussed above, a base case for coal is developed which is shown in figure 5.4. Figures 5.5 and 5.6 provide their results obtained from the simulator.



Environment: Case (Main)
Mode: Steady State

Fig. 5.4: PFD of simulation of IGCC (Coal based) power plant



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USA

Case Name:	PROJECT MAIN CASE (COAL).HSC
Unit Set:	SI
Date/Time:	Sun Aug 24 13:54:40 2014

Workbook: Case (Main)

Material Streams Fluid Pkg: All

Name	coal	steam	oxygen	fuel gas	slag
Vapour Fraction	0.3654	1.0000 *	1.0000	1.0000	0.0000
Temperature (C)	25.00 *	100.0	200.0 *	1300 *	1300
Pressure (kPa)	7000 *	101.3 *	101.3 *	7000	7000
Molar Flow (kgmole/h)	90.27	55.51	31.25	137.6	0.0000
Mass Flow (kg/h)	1000 *	1000 *	1000 *	3000	0.0000
Liquid Volume Flow (m3/h)	1.365	1.002	0.8790	4.170	0.0000
Heat Flow (kJ/h)	-1294	-1.329e+007	1.642e+005	-1.921e+007	-0.0000

Name	to mixer	to hrsg	to expander	to asu	water
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	0.0000
Temperature (C)	1402	787.4	1402	262.4	25.00 *
Pressure (kPa)	9000 *	300.0 *	9000	550.0 *	600.0 *
Molar Flow (kgmole/h)	137.6	137.6	137.6	137.6	55.51
Mass Flow (kg/h)	3000	3000	3000	3000	1000 *
Liquid Volume Flow (m3/h)	4.170	4.170	4.170	4.170	1.002
Heat Flow (kJ/h)	-1.859e+007	-2.216e+007	-1.859e+007	-2.487e+007	-1.590e+007

Name	to steam turbine	to recycler	slag-1	Steam to Gasifier	to gasifier
Vapour Fraction	1.0000 *	0.9717	1.0000	1.0000	1.0000
Temperature (C)	158.9	100.0	1296	881.2	1351
Pressure (kPa)	600.0	101.3 *	6966	7000 *	7000 *
Molar Flow (kgmole/h)	55.51	55.51	0.0000	55.51	31.25
Mass Flow (kg/h)	1000	1000	0.0000	1000	1000
Liquid Volume Flow (m3/h)	1.002	1.002	0.0000	1.002	0.8790
Heat Flow (kJ/h)	-1.319e+007	-1.335e+007	-0.0000	-1.165e+007	1.412e+006

Compositions Fluid Pkg: All

Name	coal	steam	oxygen	fuel gas	slag
Comp Mole Frac (Carbon)	0.6346 *	0.0000 *	0.0000 *	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.2747 *	0.0000 *	0.0000 *	0.1928	0.1928
Comp Mole Frac (Oxygen)	0.0907 *	0.0000 *	1.0000 *	0.0000	0.0000
Comp Mole Frac (H2O)	0.0000 *	1.0000 *	0.0000 *	0.3908	0.3908
Comp Mole Frac (CO)	0.0000 *	0.0000 *	0.0000 *	0.2467	0.2467
Comp Mole Frac (CO2)	0.0000 *	0.0000 *	0.0000 *	0.1696	0.1696
Comp Mole Frac (Methane)	0.0000 *	0.0000 *	0.0000 *	0.0000	0.0000

Name	to mixer	to hrsg	to expander	to asu	water
Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (Hydrogen)	0.1928	0.1928	0.1928	0.1928	0.0000 *
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	0.0000 *
Comp Mole Frac (H2O)	0.3908	0.3908	0.3908	0.3908	1.0000 *
Comp Mole Frac (CO)	0.2467	0.2467	0.2467	0.2467	0.0000 *
Comp Mole Frac (CO2)	0.1696	0.1696	0.1696	0.1696	0.0000 *
Comp Mole Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000 *

Name	to steam turbine	to recycler	slag-1	Steam to Gasifier	to gasifier
Comp Mole Frac (Carbon)	0.0000	0.0000	0.0000	0.0000	0.0000
Comp Mole Frac (Hydrogen)	0.0000	0.0000	0.1928	0.0000	0.0000
Comp Mole Frac (Oxygen)	0.0000	0.0000	0.0000	0.0000	1.0000
Comp Mole Frac (H2O)	1.0000	1.0000	0.3908	1.0000	0.0000
Comp Mole Frac (CO)	0.0000	0.0000	0.2467	0.0000	0.0000
Comp Mole Frac (CO2)	0.0000	0.0000	0.1696	0.0000	0.0000
Comp Mole Frac (Methane)	0.0000	0.0000	0.0000	0.0000	0.0000

Energy Streams Fluid Pkg: All

Name	q comp	Power from GT	Cooling	Power Steam Turbine	Q steam comp
Heat Flow (kJ/h)	6.237e+005	3.571e+006	-8.970e+006	1.618e+005	1.634e+006

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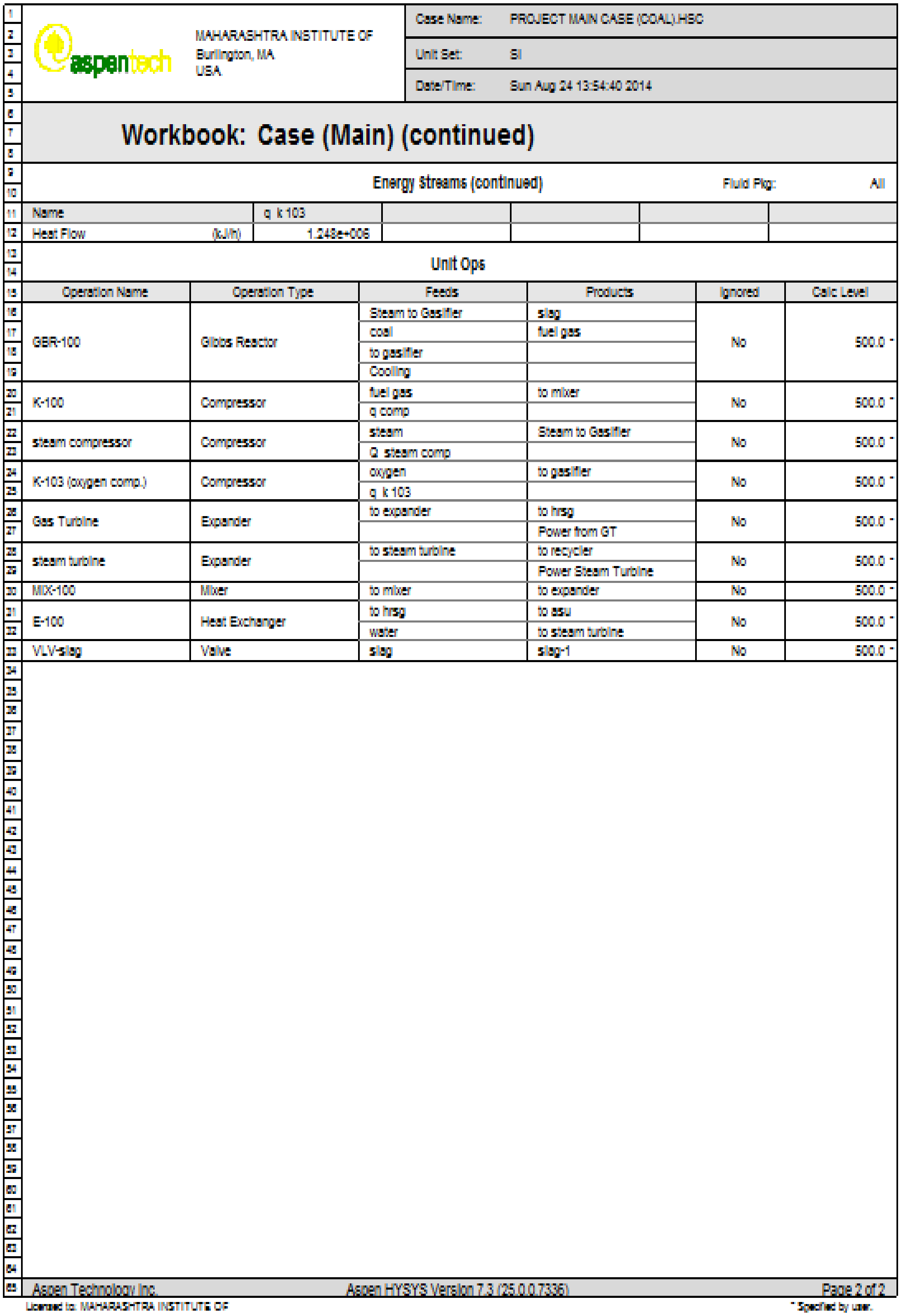
Fig. 5.5: Report with calculations of simulation of IGCC (Coal based) power plant



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Burlington, MA
USA

Case Name:	PROJECT MAIN CASE (COAL).HSC
Unit Set:	SI
Date/Time:	Sun Aug 24 13:54:40 2014

Workbook: Case (Main) (continued)

Energy Streams (continued) Fluid Pkg: All

Name		q k 103				
Heat Flow	(kJ/h)	1.248e+006				

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
GBR-100	Gibbs Reactor	Steam to Gasifier coal to gasifier Cooling	slag fuel gas	No	500.0 *
K-100	Compressor	fuel gas q comp	to mixer	No	500.0 *
steam compressor	Compressor	steam Q steam comp	Steam to Gasifier	No	500.0 *
K-103 (oxygen comp.)	Compressor	oxygen q k 103	to gasifier	No	500.0 *
Gas Turbine	Expander	to expander	to hrsg Power from GT	No	500.0 *
steam turbine	Expander	to steam turbine	to recycler Power Steam Turbine	No	500.0 *
MIX-100	Mixer	to mixer	to expander	No	500.0 *
E-100	Heat Exchanger	to hrsg water	to asu to steam turbine	No	500.0 *
VLV-slag	Valve	slag	slag-1	No	500.0 *

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Fig. 5.6: Equipment data report of simulation of IGCC (Coal based) power plant

5.6.3 Coal and Biomass

In this method, the gasification products of coal and biomass gasification are combined together in a mixer at same pressure to generate combined feed for power plant.

This concept utilizes the combined feed to generate electricity which becomes more efficient and cost effective. Figure 5.7 describes the flowsheet while figures 5.8 and 5.9 details the results obtained as reference basis.

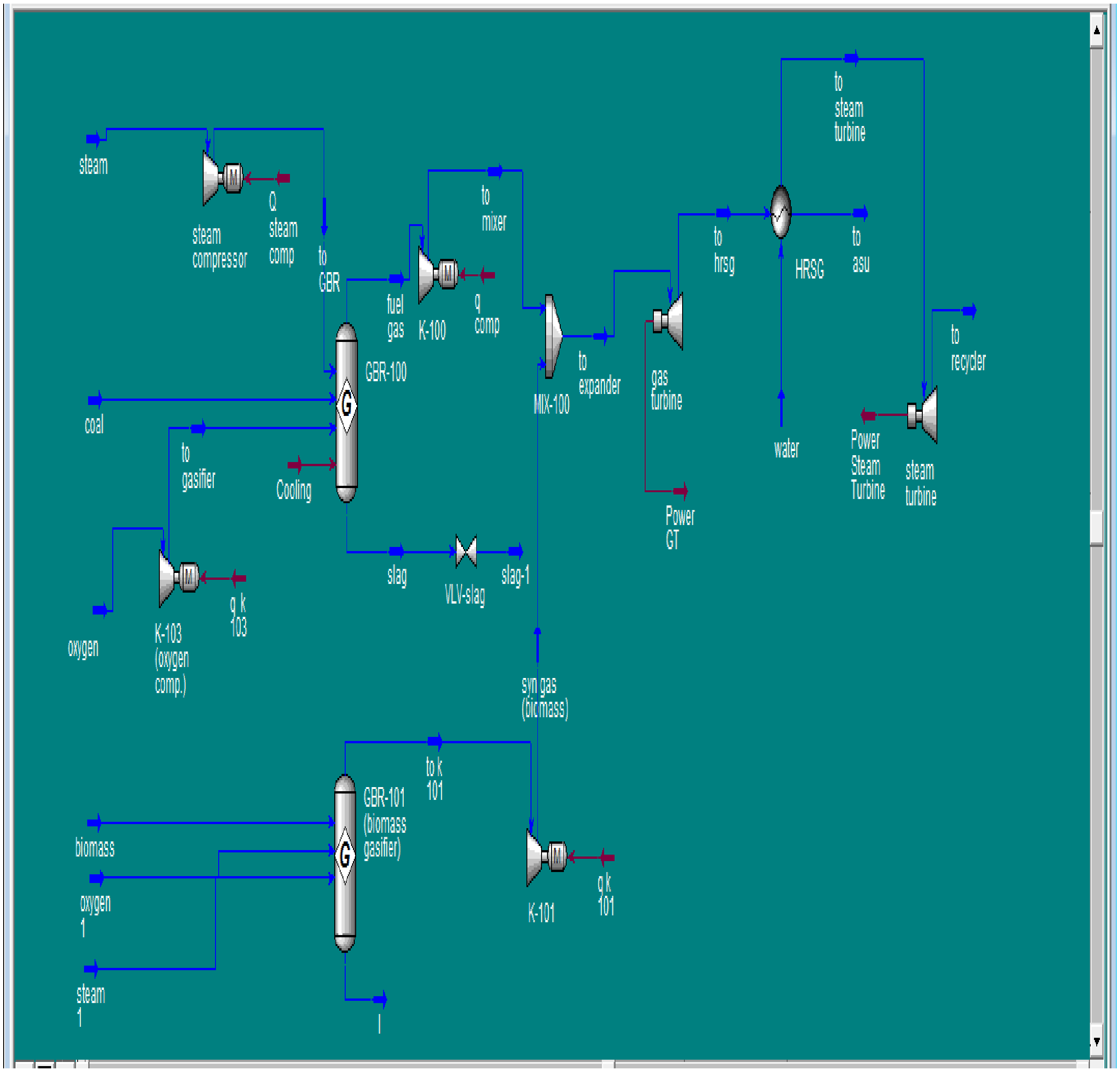
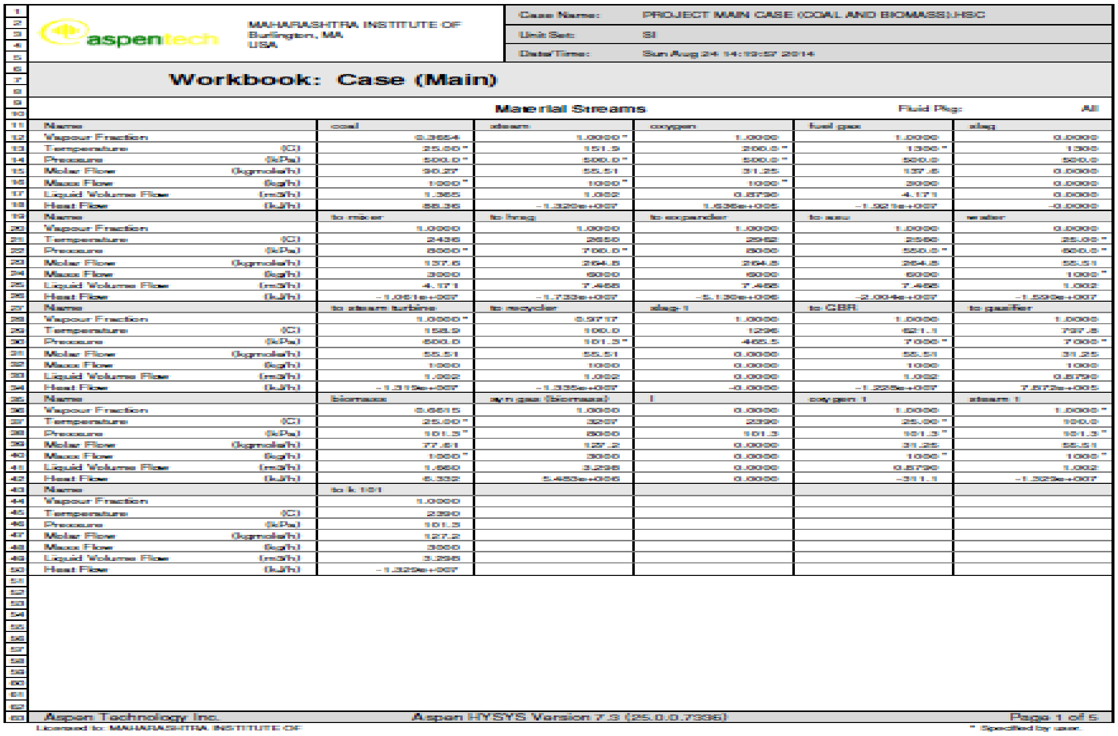


Fig. 5.7: PFD of simulation of combined feed IGCC (Coal and Biomass) power plant



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Burlington, MA
USA

Case Name:	PROJECT MAIN CASE (COAL AND BIOMASS).HSC
Unit Set:	SI
Date/Time:	Sun Aug 24 14:19:57 2014

Workbook: Case (Main)

Material Streams Fluid Pkg: All

Name		coal	steam	oxygen	fuel gas	slag
Vapour Fraction		0.3654	1.0000 *	1.0000	1.0000	0.0000
Temperature	(C)	25.00 *	151.9	200.0 *	1300 *	1300
Pressure	(kPa)	500.0 *	500.0 *	500.0 *	500.0	500.0
Molar Flow	(kgmole/h)	90.27	55.51	31.25	137.6	0.0000
Mass Flow	(kg/h)	1000 *	1000 *	1000 *	3000	0.0000
Liquid Volume Flow	(m3/h)	1.365	1.002	0.8790	4.171	0.0000
Heat Flow	(kJ/h)	88.36	-1.320e+007	1.636e+005	-1.921e+007	-0.0000
Name		to mixer	to hrsg	to expander	to asu	water
Vapour Fraction		1.0000	1.0000	1.0000	1.0000	0.0000
Temperature	(C)	2436	2650	2962	2560	25.00 *
Pressure	(kPa)	8000 *	700.0 *	8000	550.0 *	600.0 *
Molar Flow	(kgmole/h)	137.6	264.8	264.8	264.8	55.51
Mass Flow	(kg/h)	3000	6000	6000	6000	1000 *
Liquid Volume Flow	(m3/h)	4.171	7.468	7.468	7.468	1.002
Heat Flow	(kJ/h)	-1.061e+007	-1.733e+007	-5.130e+006	-2.004e+007	-1.590e+007
Name		to steam turbine	to recycler	slag 1	to GBR	to gasifier
Vapour Fraction		1.0000 *	0.9717	1.0000	1.0000	1.0000
Temperature	(C)	158.9	100.0	1296	621.1	797.8
Pressure	(kPa)	600.0	101.3 *	465.5	7000 *	7000 *
Molar Flow	(kgmole/h)	55.51	55.51	0.0000	55.51	31.25
Mass Flow	(kg/h)	1000	1000	0.0000	1000	1000
Liquid Volume Flow	(m3/h)	1.002	1.002	0.0000	1.002	0.8790
Heat Flow	(kJ/h)	-1.319e+007	-1.335e+007	-0.0000	-1.228e+007	7.872e+005
Name		biomass	syn gas (biomass)	I	oxygen 1	steam 1
Vapour Fraction		0.6615	1.0000	0.0000	1.0000	1.0000 *
Temperature	(C)	25.00 *	3207	2390	25.00 *	100.0
Pressure	(kPa)	101.3 *	8000	101.3	101.3 *	101.3 *
Molar Flow	(kgmole/h)	77.61	127.2	0.0000	31.25	55.51
Mass Flow	(kg/h)	1000 *	3000	0.0000	1000 *	1000 *
Liquid Volume Flow	(m3/h)	1.660	3.298	0.0000	0.8790	1.002
Heat Flow	(kJ/h)	6.332	5.453e+006	0.0000	-311.1	-1.323e+007
Name		to k 101				
Vapour Fraction		1.0000				
Temperature	(C)	2390				
Pressure	(kPa)	101.3				
Molar Flow	(kgmole/h)	127.2				
Mass Flow	(kg/h)	3000				
Liquid Volume Flow	(m3/h)	3.298				
Heat Flow	(kJ/h)	-1.329e+007				

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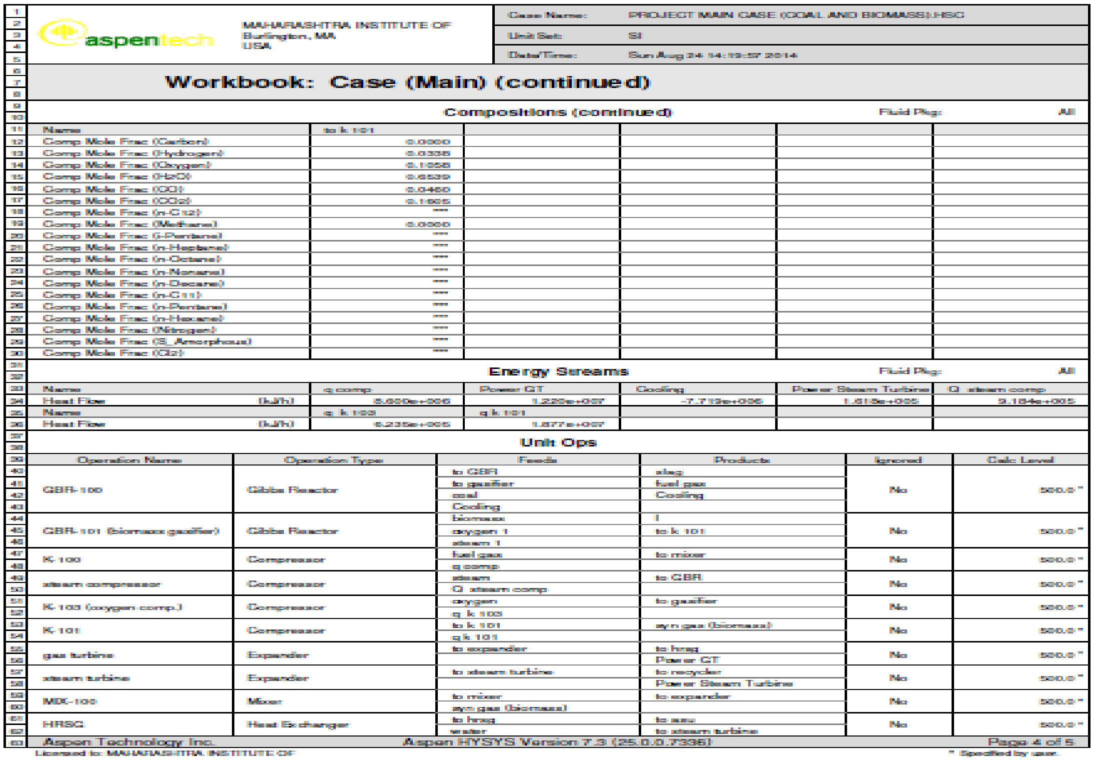
Fig. 5.8: Report with calculations of simulation of Combined feed IGCC (Coal and Biomass) power plant



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USA

Case Name:	PROJECT MAIN CASE (COAL AND BIOMASS).HSC
Unit Set:	SI
Date/Time:	Sun Aug 24 14:19:57 2014

Workbook: Case (Main) (continued)

Compositions (continued) Fluid Pkg: All

Name	to k 101				
Comp Mole Frac (Carbon)	0.0000				
Comp Mole Frac (Hydrogen)	0.0338				
Comp Mole Frac (Oxygen)	0.1058				
Comp Mole Frac (H2O)	0.6539				
Comp Mole Frac (CO)	0.0460				
Comp Mole Frac (CO2)	0.1605				
Comp Mole Frac (n-C12)	***				
Comp Mole Frac (Methane)	0.0000				
Comp Mole Frac (i-Pentane)	***				
Comp Mole Frac (n-Heptane)	***				
Comp Mole Frac (n-Octane)	***				
Comp Mole Frac (n-Nonane)	***				
Comp Mole Frac (n-Decane)	***				
Comp Mole Frac (n-C11)	***				
Comp Mole Frac (n-Pentane)	***				
Comp Mole Frac (n-Hexane)	***				
Comp Mole Frac (Nitrogen)	***				
Comp Mole Frac (S_Amorphous)	***				
Comp Mole Frac (Cl2)	***				

Energy Streams Fluid Pkg: All

Name		q comp	Power GT	Cooling	Power Steam Turbine	Q steam comp
Heat Flow	(kJ/h)	8.600e+006	1.220e+007	-7.719e+006	1.618e+005	9.184e+005
Name		q k 103	q k 101			
Heat Flow	(kJ/h)	6.235e+005	1.877e+007			

Unit Ops

Operation Name	Operation Type	Feeds	Products	Ignored	Calc Level
GBR-100	Gibbs Reactor	to GBR to gasifier coal Cooling	slag fuel gas Cooling	No	500.0 *
GBR-101 (biomass gasifier)	Gibbs Reactor	biomass oxygen 1 steam 1	I to k 101	No	500.0 *
K-100	Compressor	fuel gas q comp	to mixer	No	500.0 *
steam compressor	Compressor	steam Q steam comp	to GBR	No	500.0 *
K-103 (oxygen comp.)	Compressor	oxygen q k 103	to gasifier	No	500.0 *
K-101	Compressor	to k 101 q k 101	syn gas (biomass)	No	500.0 *
gas turbine	Expander	to expander	to hrsg Power GT	No	500.0 *
steam turbine	Expander	to steam turbine	to recycler Power Steam Turbine	No	500.0 *
MIX-100	Mixer	to mixer syn gas (biomass)	to expander	No	500.0 *
HRSG	Heat Exchanger	to hrsg water	to asu to steam turbine	No	500.0 *

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Fig. 5.9: Equipment data report of simulation of IGCC (Coal and Biomass) power plant

5.6.4 Coal and Naphtha

In this case, products from coal gasification are mixed with naphtha obtained from refinery distillation to obtain combined feed of syngas from coal and naphtha vapours.

5.6.4.1 Process description

Coal is gasified under the given conditions of temperature and pressure in the presence of steam and oxygen. The gaseous product syngas or fuel gas consisting of H_2, CO, CO_2, and H_2O is then compressed to required pressure in a compression skid and sent to the mixer where it is mixed with naphtha vapors compressed at the same pressure. The mixture of fuel gas and naphtha vapor forms the combined feed which is then fed to the IGCC power plant. The steam produced is then fed to steam turbine for further power generation. The flowsheet is shown in figure 5.10.

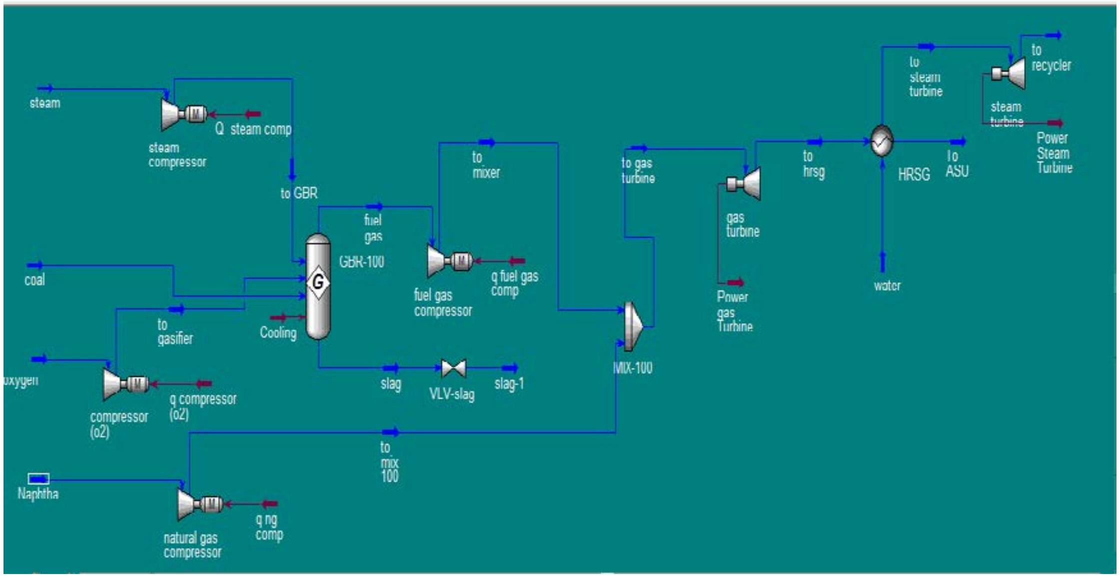


Fig. 5.10: PFD of simulation of Combined feed IGCC (Coal and Naphtha) power plant

The earlier PFD is improvised by applying a ratio controller. This ratio controller performs to regulate the gas flow to gas turbine by using Naphtha as a make-up feed to the synthesis gas generated from coal gasification in gasifier. The developed flowsheet is showcased in figure 5.11. The advantage of developing this system is that the power output is maintained by varying syngas or Naphtha, depending on availability.

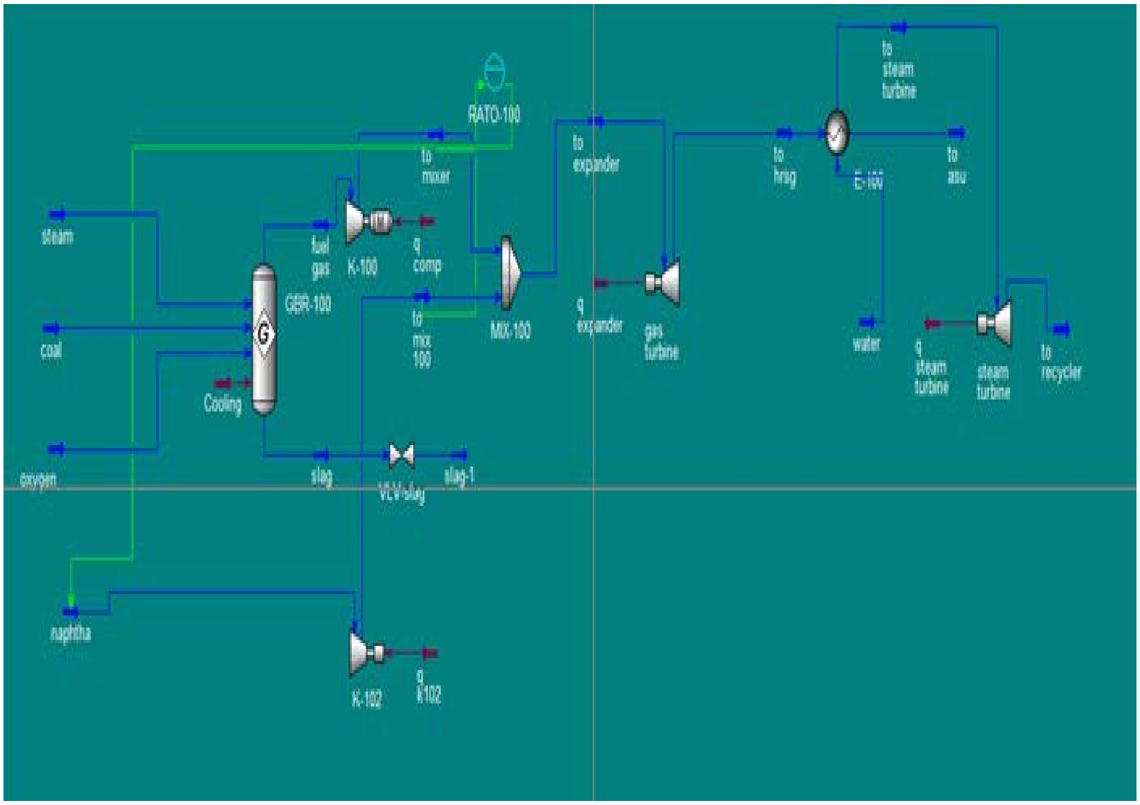


Fig. 5.11: Improvised PFD of simulation of combined feed IGCC (Coal and Naphtha) power plant with Ratio controller

5.6.5 Coal and natural gas

Similar to Coal and Naphtha combined feed, here the products from coal gasification are mixed with natural gas to obtain combined feed of syngas from coal and natural gas. Considering variations in composition of natural gas and requirement of oxygen, two flowsheets are developed. Figure 5.12 shows the direct mixing of natural gas with treated synthesis gas whereas figure 5.13 indicates addition of equilibrium reactor to stabilize natural gas using oxygen. Proper care is taken in this thesis to provide viable and robust solutions to industry for usage of combined feed options in power plants.

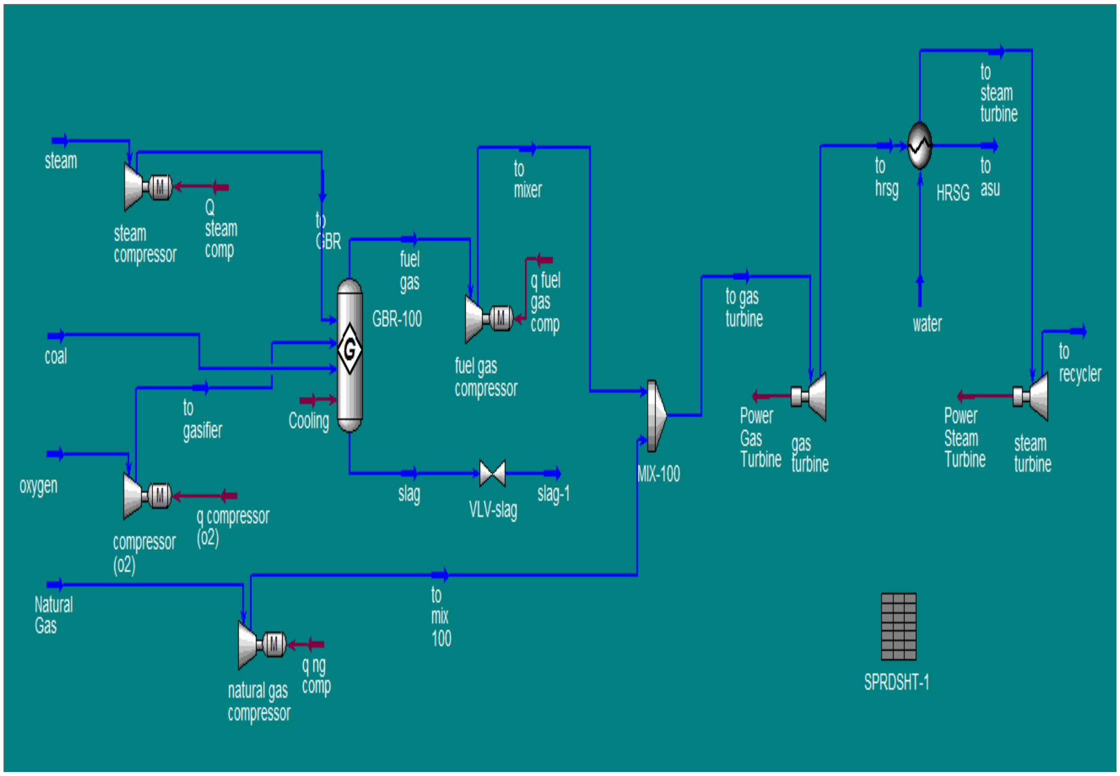


Fig. 5.12: PFD of simulation of Combined feed IGCC
(Coal and Natural gas) power plant

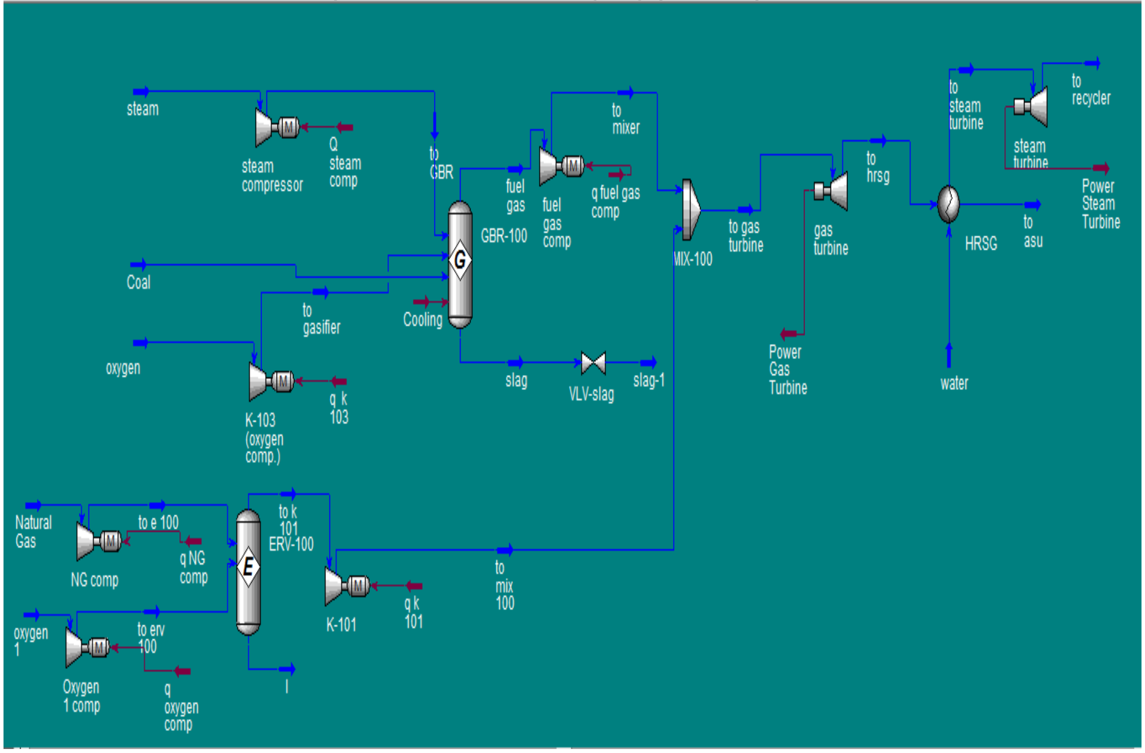


Fig. 5.13: PFD of simulation of Combined feed IGCC
(Coal and Natural gas) power plant with stabilization using Equilibrium Reactor

5.7 DESIGN SIMULATION CASE: COAL AND NATURAL GAS

Considering various fuel options for combined feed systems and their availability, we chose Coal and Natural gas combined feed IGCC power plant as the most promising combination among others. This combination is therefore chosen for detailed development and optimization. The selection of coal and natural gas as combined feed is based on the economic evaluation and market conditions in India. Indian conditions favor use of natural gas for combined feed because of greater gas reserves available indigenously and its easy as well as affordable availability. At the same time, the use of combined feed is a cost effective and efficient process. A detailed study on Natural gas based large scale power plant and its optimization is already presented in chapter 1 of this thesis.

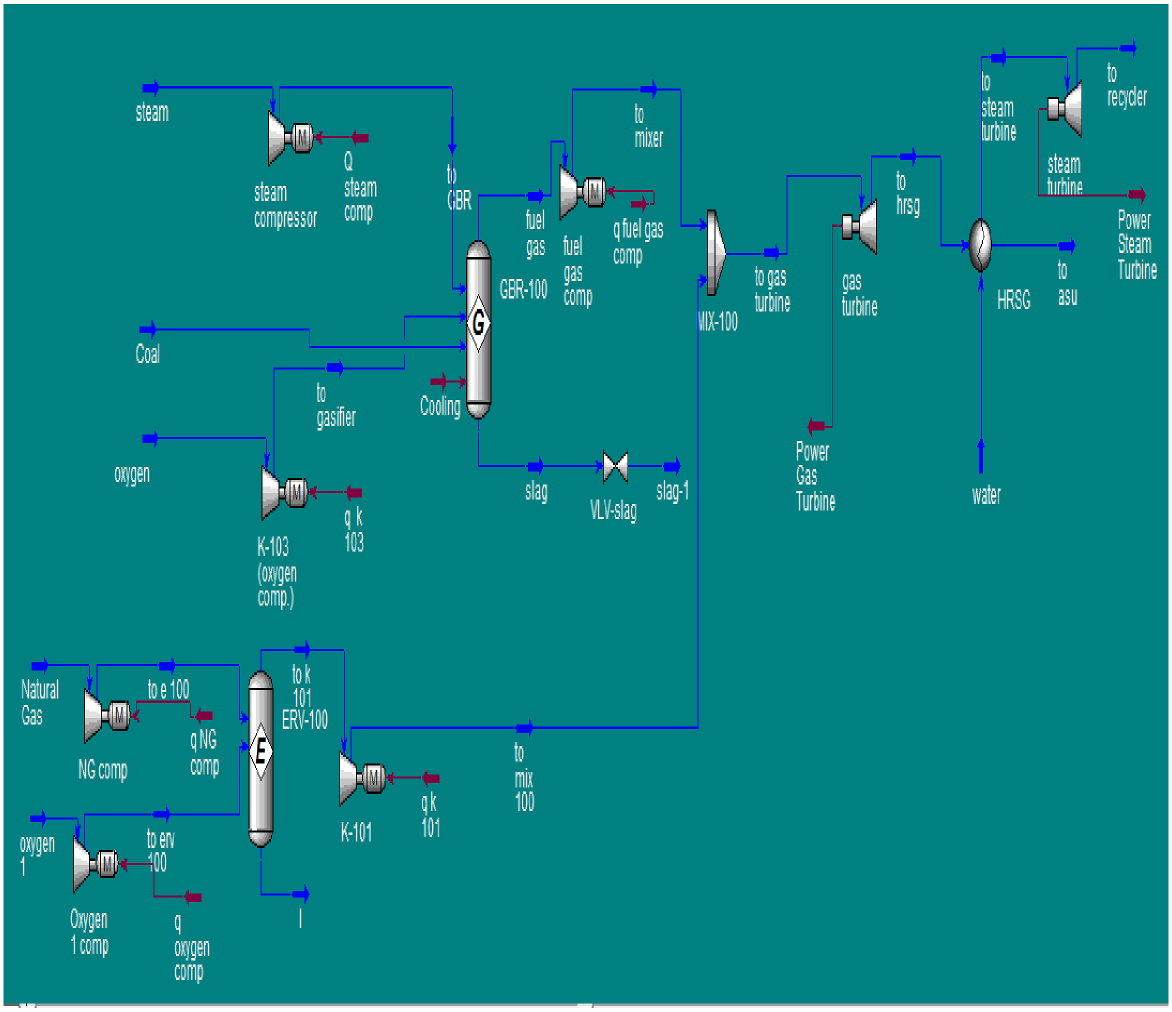


Fig. 5.14: Selected simulation of combined feed IGCC (Coal and Natural gas) power plant for optimization study

5.8 DEVELOPMENT OF DESIGN CASE STUDY FOR OPTIMIZATION WITH KEY VARIABLES

The step wise design of selected flowsheet in the simulator Aspen HYSYS® is discussed below.

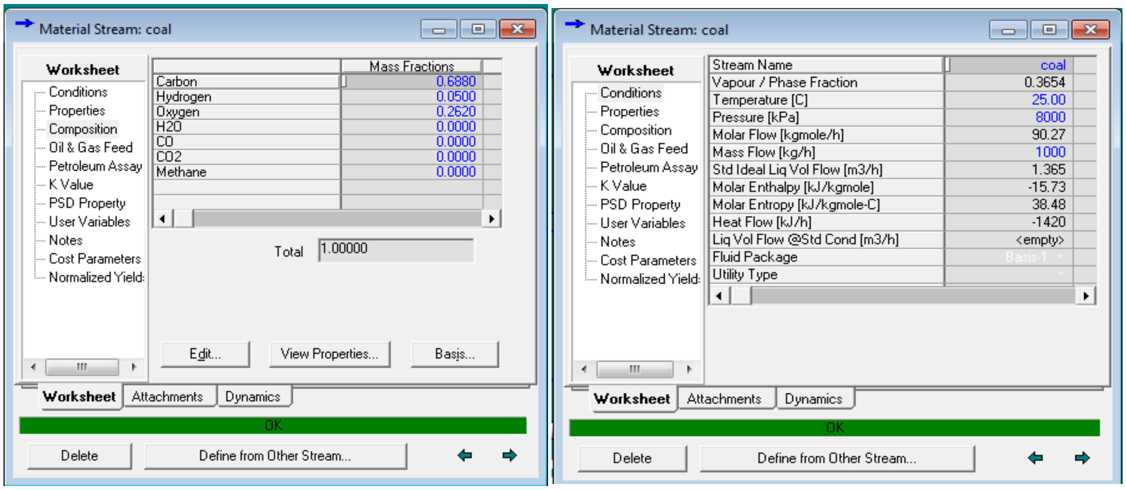
5.8.1 Process Description

Feed:

- Coal
- Steam
- Oxygen

Feed is fed to the gasifier which is a fixed bed gasifier, in which partial combustion takes place and product gases are generated. Products from the gasifier are in the vapour form and at very high temperature. The syngas is then compressed to very high pressure and sent to the mixer where natural gas is added at same pressure to generate a combined feed which is sent to the gas turbine for power generation. The gas coming out of gas turbine goes to heat recovery steam generator which is a heat exchanger and generates steam by utilizing heat from the flue gas of gas turbine. Figure 5.15 shows the coal composition entered in the simulator while figures 5.16 and 5.17 show gasifier conditions and compressor details.

5.8.1.1 Coal Feed



Material Stream: coal

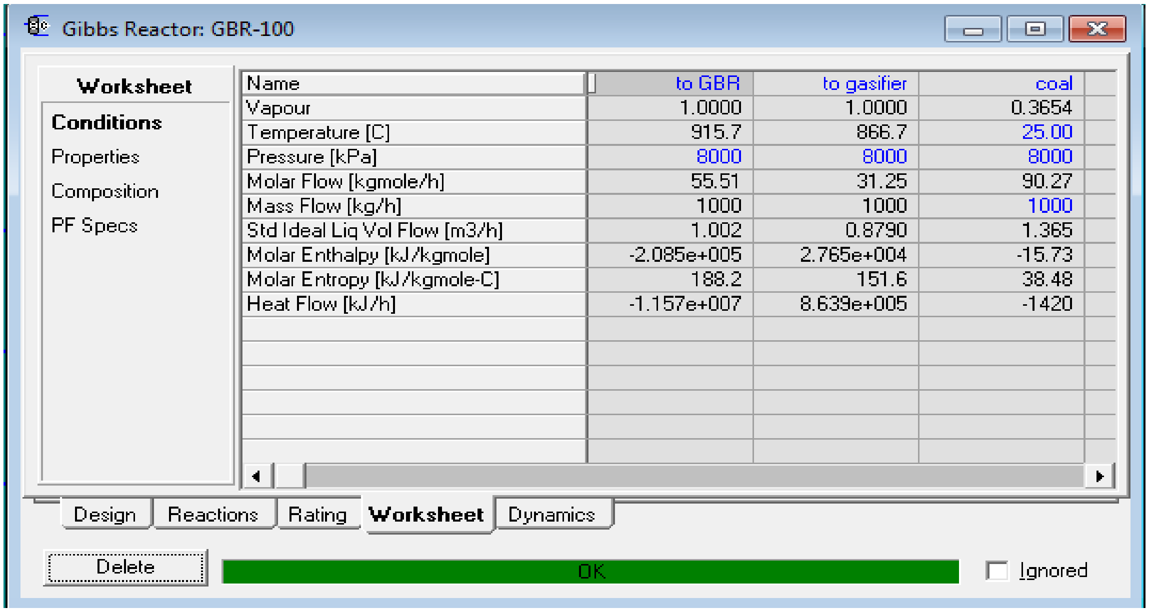
	Mass Fractions
Carbon	0.6880
Hydrogen	0.0500
Oxygen	0.2620
H2O	0.0000
CO	0.0000
CO2	0.0000
Methane	0.0000

Total 1.00000

Material Stream: coal

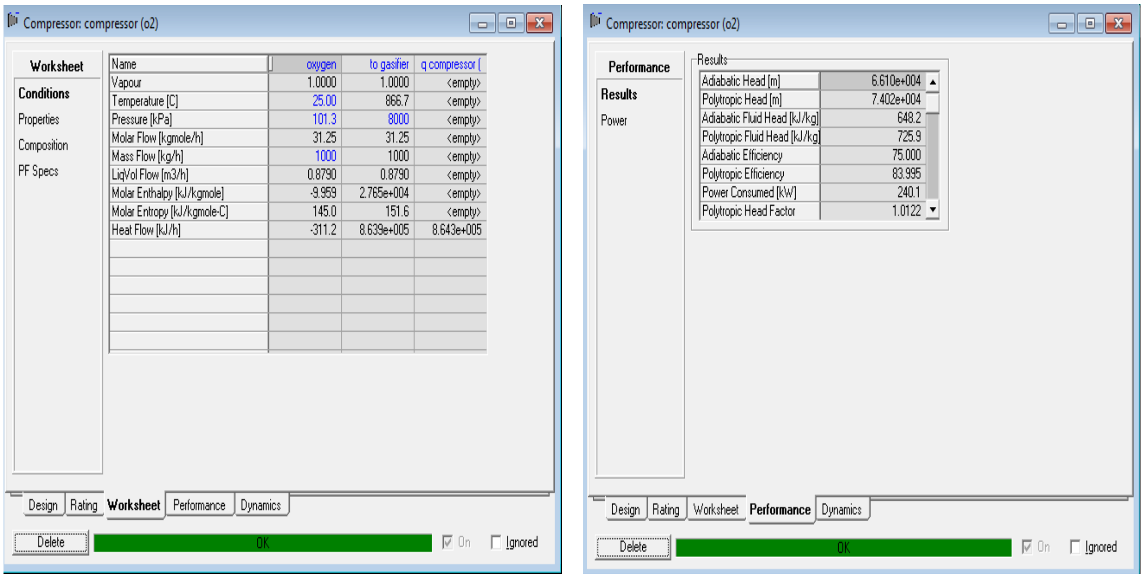
Stream Name	coal
Vapour / Phase Fraction	0.3654
Temperature [C]	25.00
Pressure [kPa]	8000
Molar Flow [kgmole/h]	90.27
Mass Flow [kg/h]	1000
Std Ideal Liq Vol Flow [m3/h]	1.365
Molar Enthalpy [kJ/kgmole]	-15.73
Molar Entropy [kJ/kgmole-C]	38.48
Heat Flow [kJ/h]	-1420
Liq Vol Flow @Std Cond [m3/h]	<empty>
Fluid Package	Basis-1
Utility Type	

Fig. 5.15: Composition of coal and feed stream details



Name	to GBR	to gasifier	coal
Vapour	1.0000	1.0000	0.3654
Temperature [C]	915.7	866.7	25.00
Pressure [kPa]	8000	8000	8000
Molar Flow [kgmole/h]	55.51	31.25	90.27
Mass Flow [kg/h]	1000	1000	1000
Std Ideal Liq Vol Flow [m3/h]	1.002	0.8790	1.365
Molar Enthalpy [kJ/kgmole]	-2.085e+005	2.765e+004	-15.73
Molar Entropy [kJ/kgmole-C]	188.2	151.6	38.48
Heat Flow [kJ/h]	-1.157e+007	8.639e+005	-1420

Fig. 5.16: Gasifier conditions, modeled as Gibbs Reactor



Name	oxygen	to gasifier	q compressor (
Vapour	1.0000	1.0000	<empty>
Temperature [C]	25.00	866.7	<empty>
Pressure [kPa]	101.3	8000	<empty>
Molar Flow [kgmole/h]	31.25	31.25	<empty>
Mass Flow [kg/h]	1000	1000	<empty>
LiqVol Flow [m3/h]	0.8790	0.8790	<empty>
Molar Enthalpy [kJ/kgmole]	-9.959	2.765e+004	<empty>
Molar Entropy [kJ/kgmole-C]	145.0	151.6	<empty>
Heat Flow [kJ/h]	-311.2	8.639e+005	8.643e+005

Results

Adiabatic Head [m]	6.610e+004
Polytropic Head [m]	7.402e+004
Adiabatic Fluid Head [kJ/kg]	648.2
Polytropic Fluid Head [kJ/kg]	725.9
Adiabatic Efficiency	75.000
Polytropic Efficiency	83.995
Power Consumed [kW]	240.1
Polytropic Head Factor	1.0122

Fig. 5.17: Compression data for Syngas

5.8.1.2 Natural gas

Natural gas is blended with the syngas from the gasifier with the purpose of increasing the calorific value of feed. The natural gas feed is first fed to an equilibrium reactor where CO and H_2 rich gas is produced. This gas is compressed and sent to the gas mixer unit. Figures 5.18 and 5.19 indicate the stabilizing of natural gas by partial combustion and its compression in compressor.

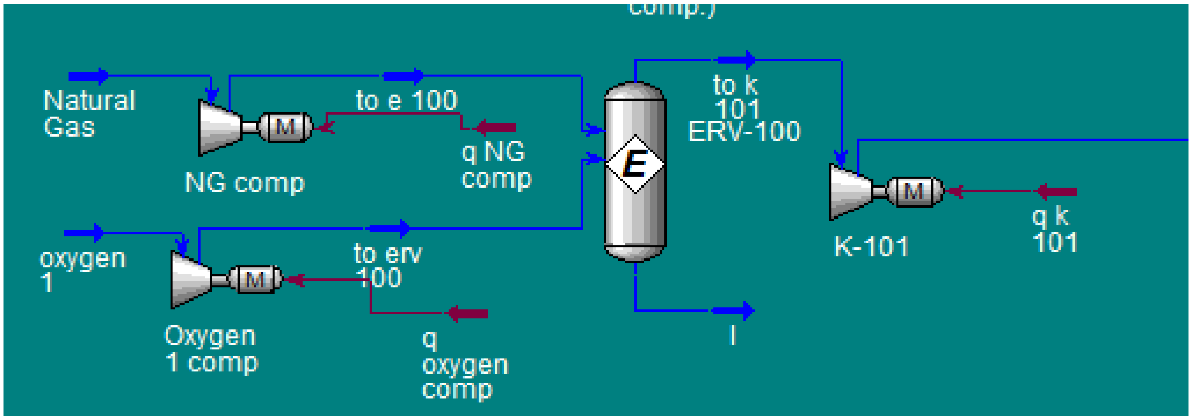
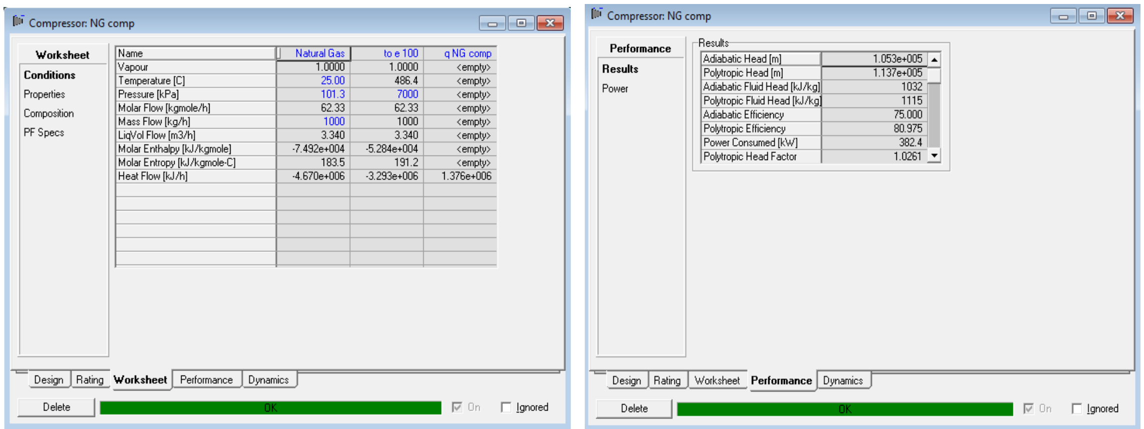


Fig. 5.18: PFD of Partial Combustion of Natural Gas



Compressor: NG comp

Worksheet

Conditions
Properties
Composition
PF Specs

Name	Natural Gas	to e 100	q NG comp
Vapour	1.0000	1.0000	<empty>
Temperature [C]	25.00	486.4	<empty>
Pressure [kPa]	101.3	7000	<empty>
Molar Flow [kgmole/h]	62.33	62.33	<empty>
Mass Flow [kg/h]	1000	1000	<empty>
LiqVol Flow [m3/h]	3.340	3.340	<empty>
Molar Enthalpy [kJ/kgmole]	-7.492e+004	-5.284e+004	<empty>
Molar Entropy [kJ/kgmole-C]	183.5	191.2	<empty>
Heat Flow [kJ/h]	-4.670e+006	-3.293e+006	1.376e+006

Compressor: NG comp

Performance

Results
Power

Results

Adiabatic Head [m]	1.053e+005
Polytropic Head [m]	1.137e+005
Adiabatic Fluid Head [kJ/kg]	1032
Polytropic Fluid Head [kJ/kg]	1115
Adiabatic Efficiency	75.000
Polytropic Efficiency	80.975
Power Consumed [kW]	382.4
Polytropic Head Factor	1.0261

Fig. 5.19: Compression Data of Natural Gas

5.8.1.3 Blending of Syngas and Natural Gas

Mixing of syngas and natural gas after compression at same pressure is performed. The blending flowsheet and blending data are shown in figures 5.20 and 5.21.

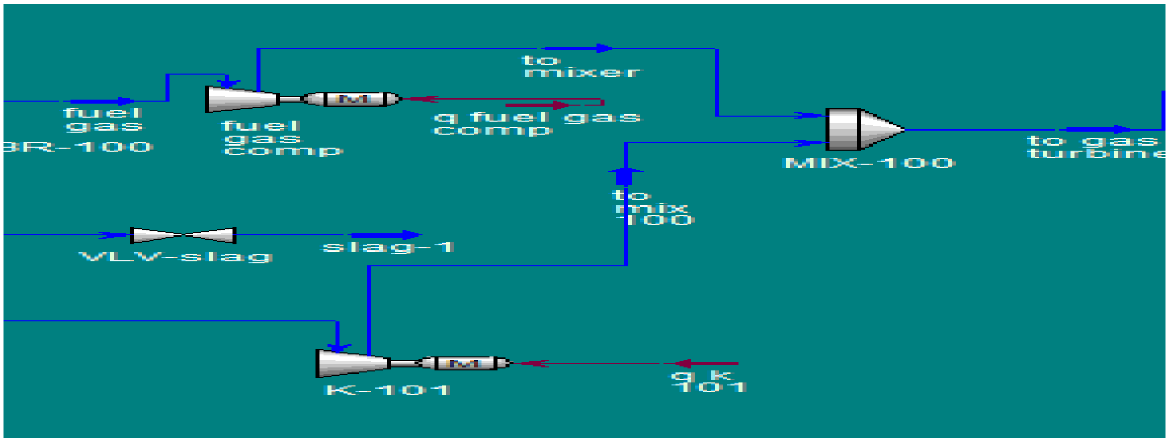
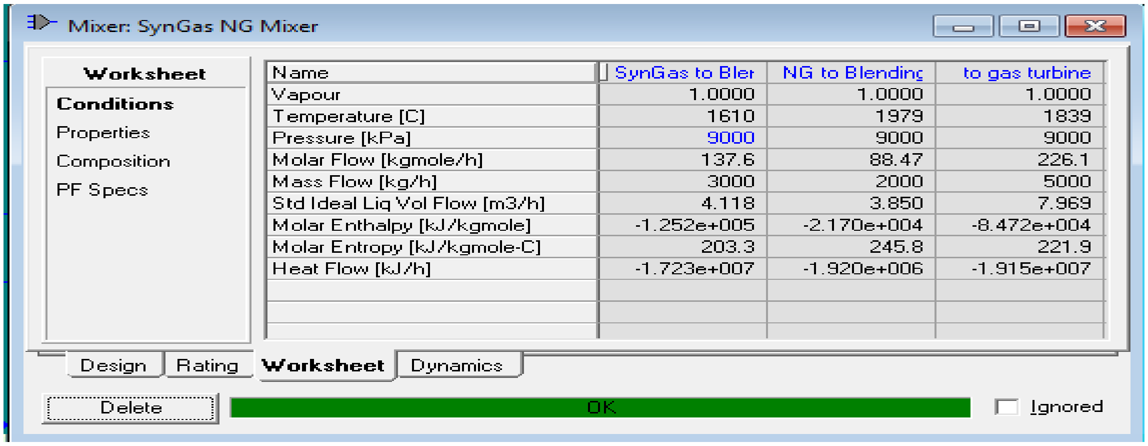


Fig. 5.20: PFD of syngas and Natural Gas blending.



Name	SynGas to Bler	NG to Blending	to gas turbine
Vapour	1.0000	1.0000	1.0000
Temperature [C]	1610	1979	1839
Pressure [kPa]	9000	9000	9000
Molar Flow [kgmole/h]	137.6	88.47	226.1
Mass Flow [kg/h]	3000	2000	5000
Std Ideal Liq Vol Flow [m3/h]	4.118	3.850	7.969
Molar Enthalpy [kJ/kgmole]	-1.252e+005	-2.170e+004	-8.472e+004
Molar Entropy [kJ/kgmole-C]	203.3	245.8	221.9
Heat Flow [kJ/h]	-1.723e+007	-1.920e+006	-1.915e+007

Fig. 5.21: Natural gas and syn gas blending data

5.8.1.4 Gas Turbine

The combined feed at very high pressure is sent to the gas turbine for power generation. The flowsheet and gas turbine details are shown in figures 5.22 and 5.23.

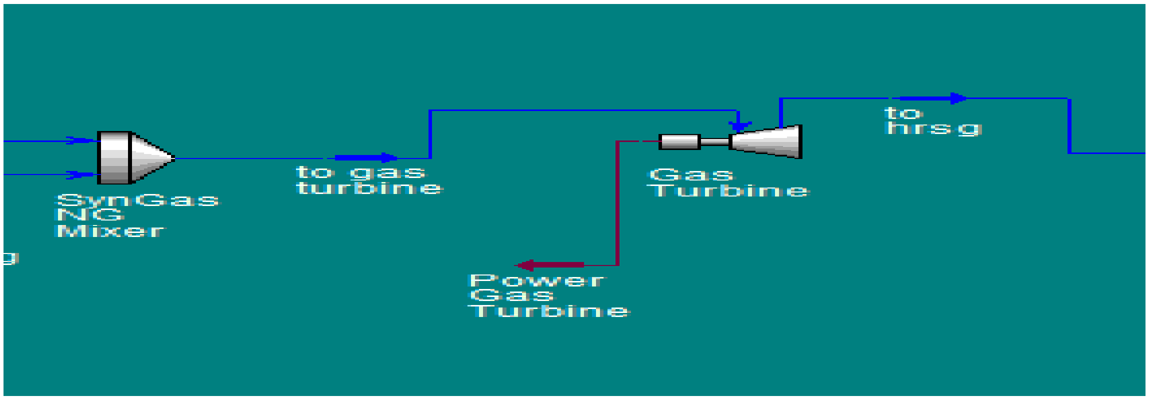
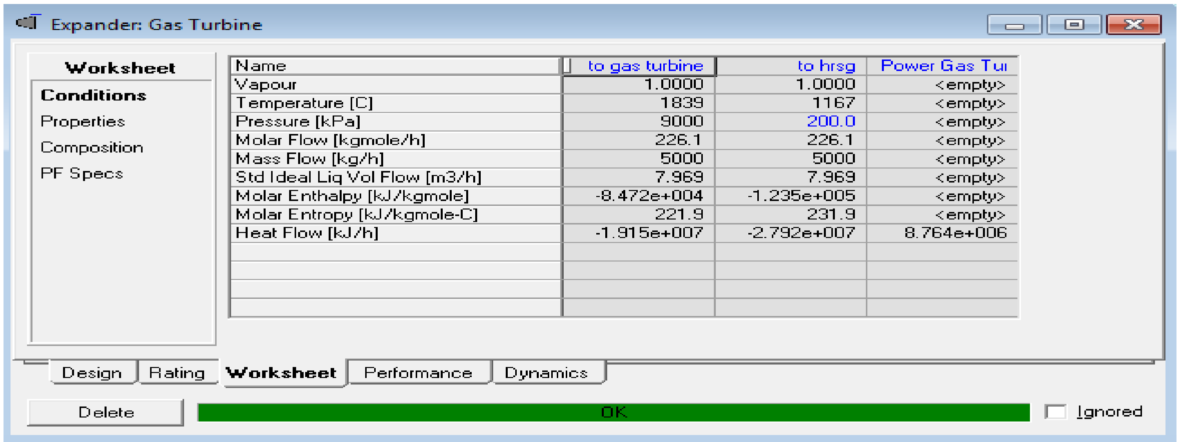


Fig. 5.22: PFD of Gas Turbine



Name	to gas turbine	to hrsg	Power Gas Tur
Vapour	1.0000	1.0000	<empty>
Temperature [C]	1839	1167	<empty>
Pressure [kPa]	9000	200.0	<empty>
Molar Flow [kgmole/h]	226.1	226.1	<empty>
Mass Flow [kg/h]	5000	5000	<empty>
Std Ideal Liq Vol Flow [m3/h]	7.969	7.969	<empty>
Molar Enthalpy [kJ/kgmole]	-8.472e+004	-1.235e+005	<empty>
Molar Entropy [kJ/kgmole-C]	221.9	231.9	<empty>
Heat Flow [kJ/h]	-1.915e+007	-2.792e+007	8.764e+006

Fig. 5.23: Conditions in a Gas Turbine

5.8.1.5 Heat Recovery Steam Generator (HRSG)

Heat recovery steam generation is the process of recovering unused heat of the flue gas coming out of gas turbine for further power generation. The PFD, HRSG design details and process conditions are shown in figures 5.24 through 5. 26.

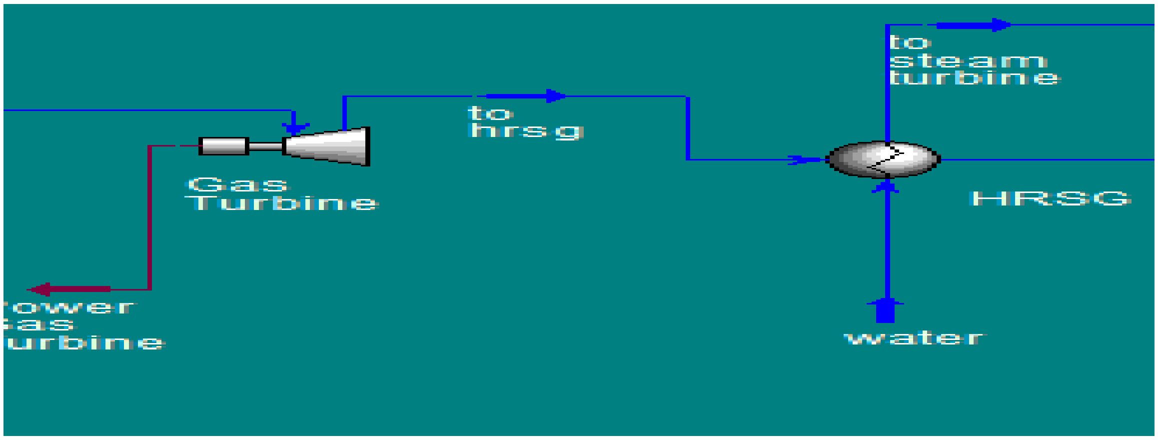
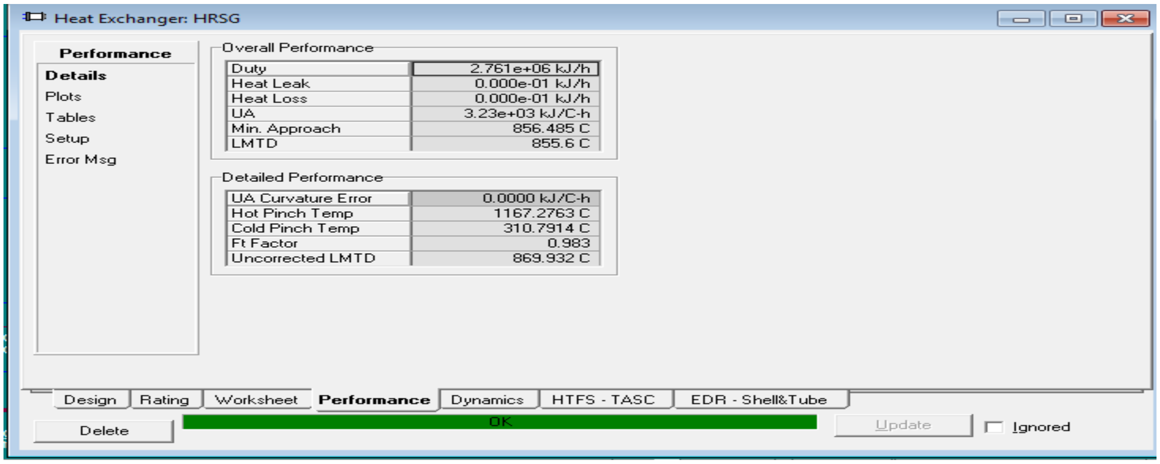


Fig. 5.24: PFD of Heat Recovery Steam Generator



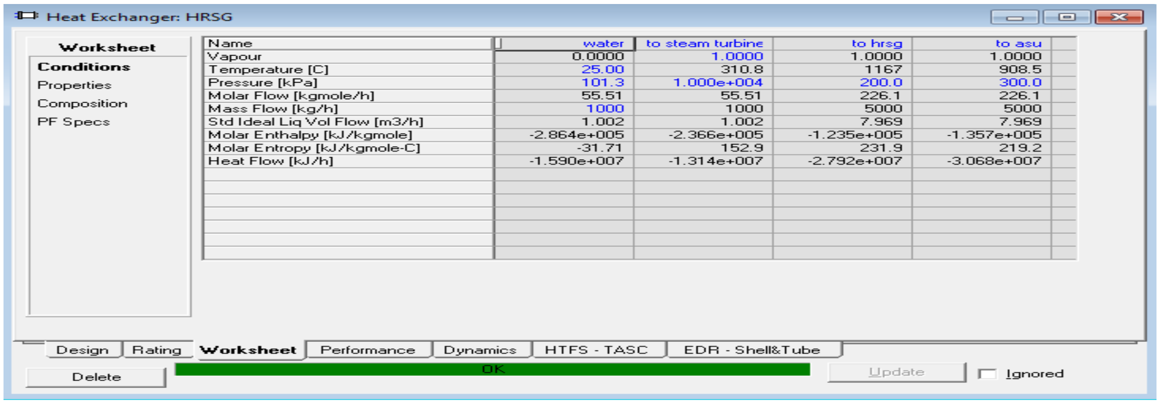
Overall Performance

Duty	2.761e+06 kJ/h
Heat Leak	0.000e-01 kJ/h
Heat Loss	0.000e-01 kJ/h
UA	3.23e+03 kJ/C-h
Min. Approach	856.485 C
LMTD	855.6 C

Detailed Performance

UA Curvature Error	0.0000 kJ/C-h
Hot Pinch Temp	1167.2763 C
Cold Pinch Temp	310.7914 C
Ft Factor	0.983
Uncorrected LMTD	869.932 C

Fig. 5.25: HRSG design details



Name	water	to steam turbine	to hrsg	to asu
Vapour	0.0000	1.0000	1.0000	1.0000
Temperature [C]	25.00	310.8	1167	908.5
Pressure [kPa]	101.3	1.000e+004	200.0	300.0
Molar Flow [kgmole/h]	55.51	55.51	226.1	226.1
Mass Flow [kg/h]	1000	1000	5000	5000
Std Ideal Liq Vol Flow [m3/h]	1.002	1.002	7.969	7.969
Molar Enthalpy [kJ/kgmole]	-2.864e+005	-2.366e+005	-1.235e+005	-1.357e+005
Molar Entropy [kJ/kgmole-C]	-31.71	152.9	231.9	219.2
Heat Flow [kJ/h]	-1.590e+007	-1.314e+007	-2.792e+007	-3.068e+007

Fig. 5.26: HRSG process conditions

5.8.1.6 Steam Turbine

The steam generated in the HRSG is fed to the steam turbine for further power generation. Figure 5.27 shows the flowsheet part for steam turbine whereas figure 5.28 provides steam turbine details.

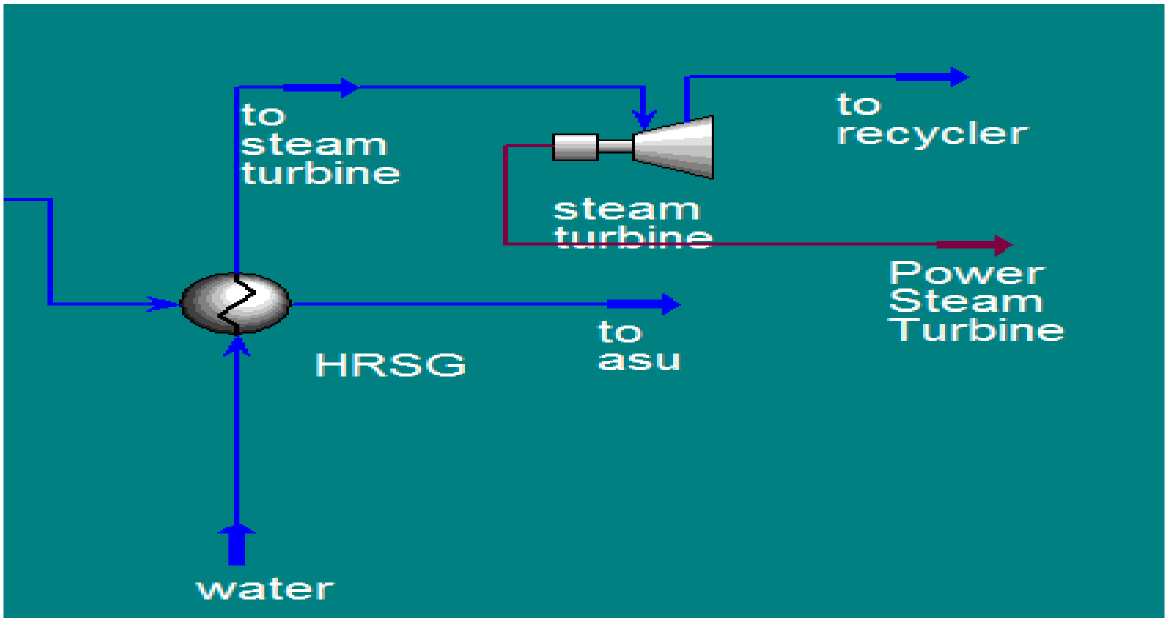
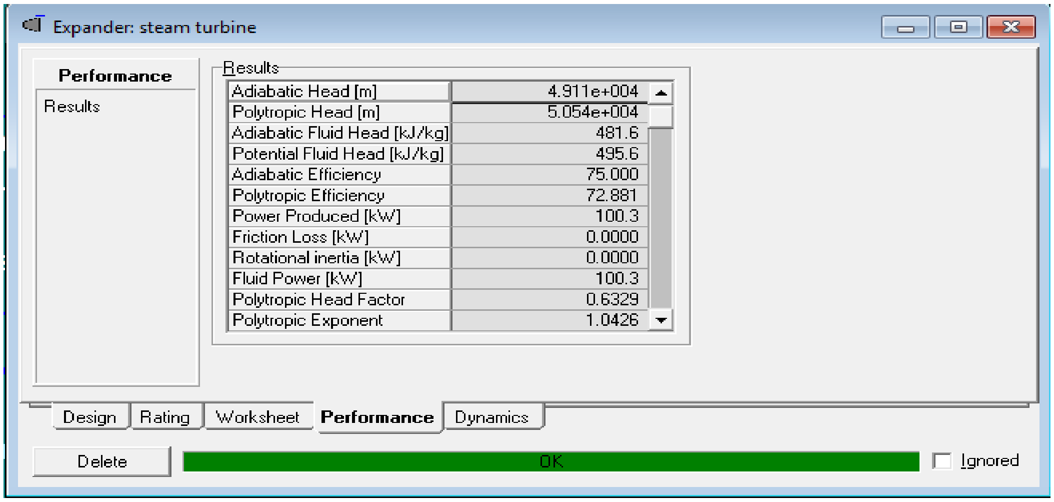


Fig. 5.27: PFD of Steam Turbine



Results

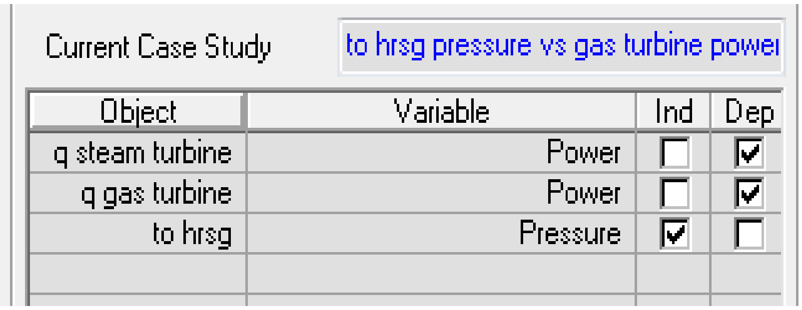
Adiabatic Head [m]	4.911e+004
Polytropic Head [m]	5.054e+004
Adiabatic Fluid Head [kJ/kg]	481.6
Potential Fluid Head [kJ/kg]	495.6
Adiabatic Efficiency	75.000
Polytropic Efficiency	72.881
Power Produced [kW]	100.3
Friction Loss [kW]	0.0000
Rotational inertia [kW]	0.0000
Fluid Power [kW]	100.3
Polytropic Head Factor	0.6329
Polytropic Exponent	1.0426

Fig. 5.28: Steam Turbine data details

Now, with the finalized and fully developed design case study, we have chosen various parameters to analyze their effect on performance. These optimization studies are carried out, which are explained in details in section 5.9 below.

5.9 PARAMETRIC OPTIMIZATION

5.9.1 Case 1: Effect of pressure drop across gas turbine on power generated in gas turbine

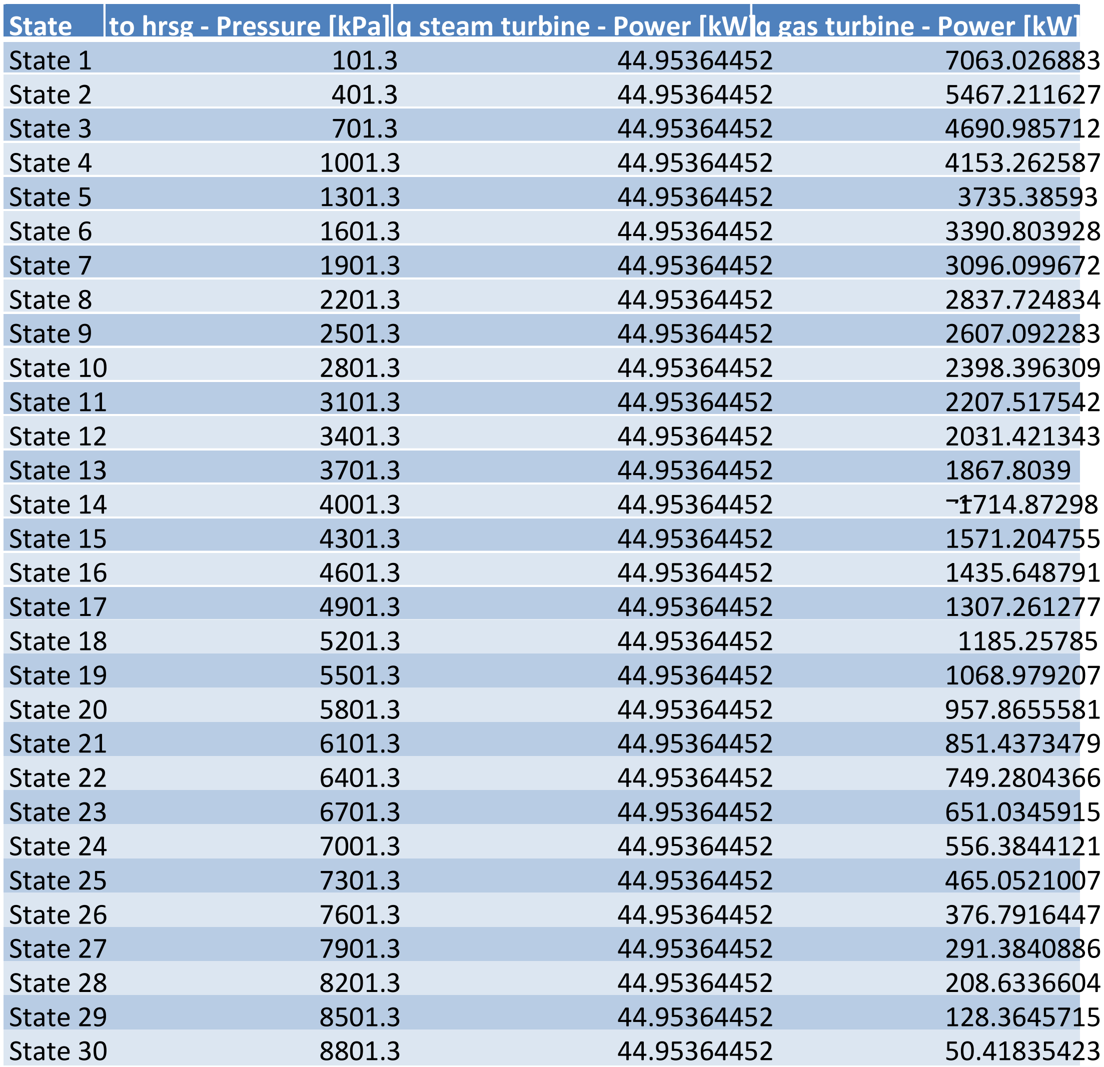


Current Case Study: to hrsg pressure vs gas turbine powe

Object	Variable	Ind	Dep
q steam turbine	Power	☐	☑
q gas turbine	Power	☐	☑
to hrsg	Pressure	☑	☐

Fig. 5.29: Selection of dependent and independent variables

Table 5.3: Comparison of pressure drop across gas turbine with power generated in gas turbine



State	to hrsg - Pressure [kPa]	q steam turbine - Power [kW	q gas turbine - Power [kW
State 1	101.3	44.95364452	7063.026883
State 2	401.3	44.95364452	5467.211627
State 3	701.3	44.95364452	4690.985712
State 4	1001.3	44.95364452	4153.262587
State 5	1301.3	44.95364452	3735.38593
State 6	1601.3	44.95364452	3390.803928
State 7	1901.3	44.95364452	3096.099672
State 8	2201.3	44.95364452	2837.724834
State 9	2501.3	44.95364452	2607.092283
State 10	2801.3	44.95364452	2398.396309
State 11	3101.3	44.95364452	2207.517542
State 12	3401.3	44.95364452	2031.421343
State 13	3701.3	44.95364452	1867.8039
State 14	4001.3	44.95364452	1714.87298
State 15	4301.3	44.95364452	1571.204755
State 16	4601.3	44.95364452	1435.648791
State 17	4901.3	44.95364452	1307.261277
State 18	5201.3	44.95364452	1185.25785
State 19	5501.3	44.95364452	1068.979207
State 20	5801.3	44.95364452	957.8655581
State 21	6101.3	44.95364452	851.4373479
State 22	6401.3	44.95364452	749.2804366
State 23	6701.3	44.95364452	651.0345915
State 24	7001.3	44.95364452	556.3844121
State 25	7301.3	44.95364452	465.0521007
State 26	7601.3	44.95364452	376.7916447
State 27	7901.3	44.95364452	291.3840886
State 28	8201.3	44.95364452	208.6336604
State 29	8501.3	44.95364452	128.3645715
State 30	8801.3	44.95364452	50.41835423

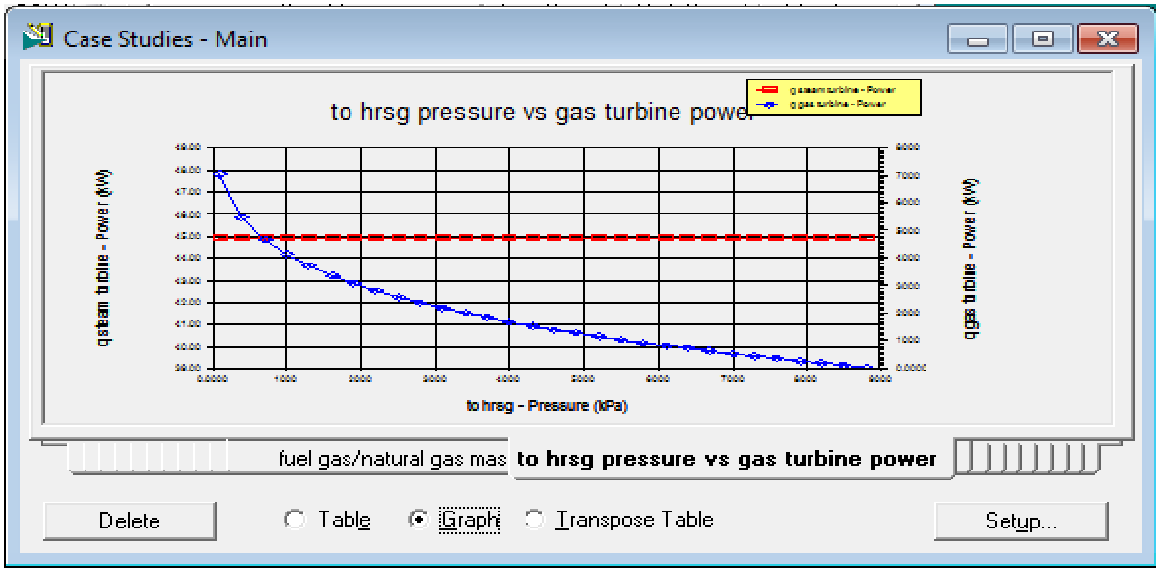


Fig. 5.30: Plot of pressure drop in gas turbine and gas turbine power generated

Figure 5.29 shows the selection of variables. Table 5.3 indicates the data generated to conduct the present case study while figure 5.30 shows the results indicating the effect of gas turbine pressure drop on power produced.

Conclusion

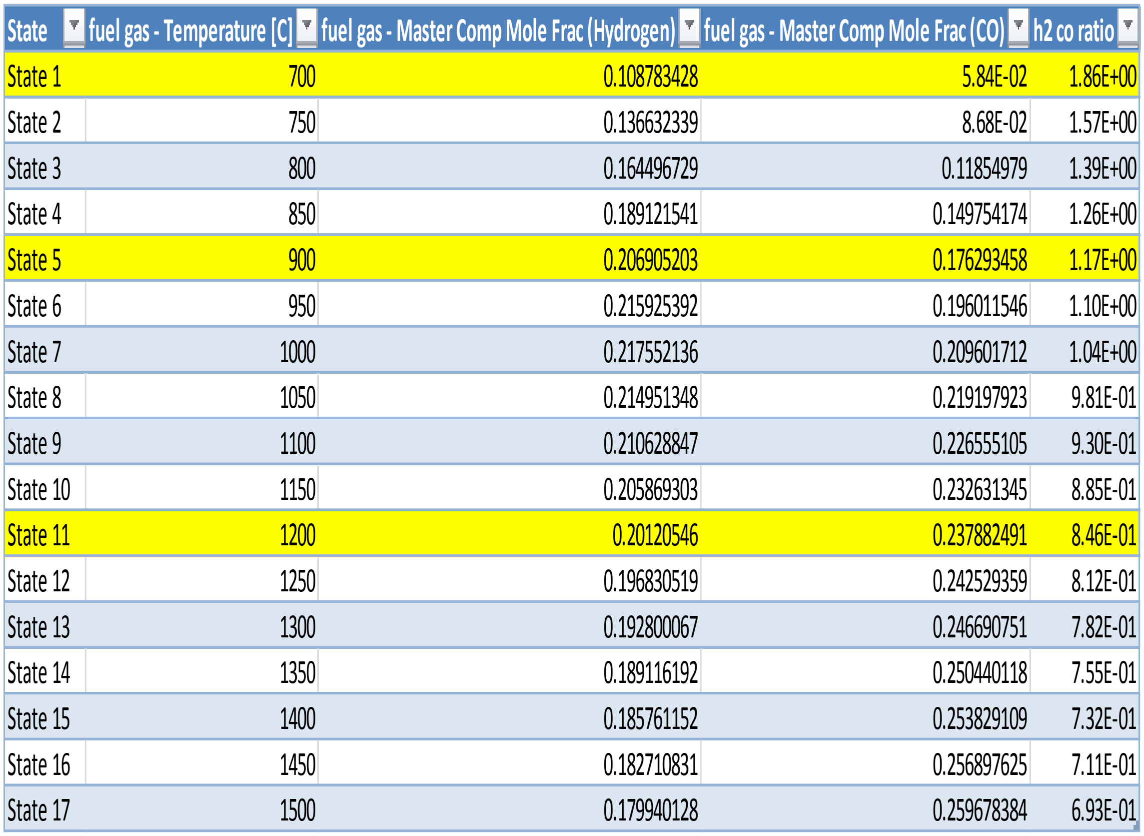
As the pressure drop across gas turbine increases, the power generated in gas turbine also increases.

5.9.1 Case 2: This case is a comparison of H_2 to CO ratio in fuel gas produced from gasifier and temperature of fuel gas.

The calorific value of syn gas increases with increase in H_2 to CO ratio, and this case study helps in obtaining temperature of fuel gas for which we get maximum H_2 to CO ratio. The optimum temperature obtained can be taken as base case for further steps.

Table 5.4 and figure 5.31 elaborate on the results generated by the present case study.

Table 5.4: Data of temperature of fuel gas and its effect on H_2 / CO ratio



State	fuel gas - Temperature [C]	fuel gas - Master Comp Mole Frac (Hydrogen)	fuel gas - Master Comp Mole Frac (CO)	h2 co ratio
State 1	700	0.108783428	5.84E-02	1.86E+00
State 2	750	0.136632339	8.68E-02	1.57E+00
State 3	800	0.164496729	0.11854979	1.39E+00
State 4	850	0.189121541	0.149754174	1.26E+00
State 5	900	0.206905203	0.176293458	1.17E+00
State 6	950	0.215925392	0.196011546	1.10E+00
State 7	1000	0.217552136	0.209601712	1.04E+00
State 8	1050	0.214951348	0.219197923	9.81E-01
State 9	1100	0.210628847	0.226555105	9.30E-01
State 10	1150	0.205869303	0.232631345	8.85E-01
State 11	1200	0.20120546	0.237882491	8.46E-01
State 12	1250	0.196830519	0.242529359	8.12E-01
State 13	1300	0.192800067	0.246690751	7.82E-01
State 14	1350	0.189116192	0.250440118	7.55E-01
State 15	1400	0.185761152	0.253829109	7.32E-01
State 16	1450	0.182710831	0.256897625	7.11E-01
State 17	1500	0.179940128	0.259678384	6.93E-01

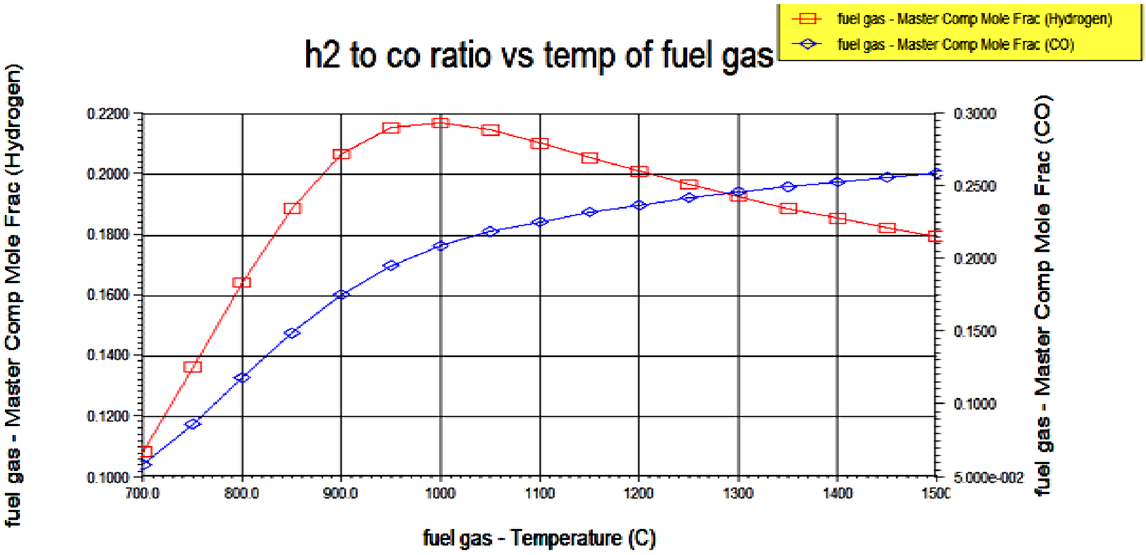


Fig. 5.31: Plot of temperature of fuel gas and its effect on H_2 / CO ratio

Conclusion

As temperature of fuel gas increases, the H_2 to CO ratio decreases. But at lower temperatures, the power production is affected.

5.9.3 Case 3: The effect of fuel gas temperature and mixer feed stream pressure on power produced is studied.

- To mixer pressure is the pressure of the feed to gas turbine after blending
- Independent variable- fuel gas temperature and to mixer pressure
- Dependent variable - power generated in the gas turbine

Table 5.5 provides optimized data generated in present study and figure 5.32 provides surface plot to represent the voluminous data to derive conclusions.

Table 5.5: Optimization data for fuel gas temperature, mixer pressure stream and power produced in gas turbine

State	Fuel gas temperature(^{0}C)	To mixer pressure (kPa)	Power generated in gas turbine (KW)
State 1	100.000000000000	101.324996582814	-142.466604404744
State 2	100.000000000000	1114.57496241096	73.4347160806774
State 3	100.000000000000	2127.82492823910	65.9761943619251
State 4	100.000000000000	3141.07489406725	109.943026962765
State 5	100.000000000000	4154.32485989539	143.229621053100
State 6	100.000000000000	5167.57482572354	173.795145493545
State 7	100.000000000000	6180.82479155168	201.480463478865
State 8	100.000000000000	7194.07475737983	226.069966674677
State 9	100.000000000000	8207.32472320797	248.265907421383
State 10	100.000000000000	9220.57468903612	268.565354018230
State 11	200.000000000000	101.324996582814	-272.086913696065
State 12	200.000000000000	1114.57496241096	137.046660420667
State 13	200.000000000000	2127.82492823910	246.592360255378
State 14	200.000000000000	3141.07489406725	311.189026781442
State 15	200.000000000000	4154.32485989539	356.364602838232
State 16	200.000000000000	5167.57482572354	390.608299295982
State 17	200.000000000000	6180.82479155168	417.832182678043
State 18	200.000000000000	7194.07475737983	440.182635669311
State 19	200.000000000000	8207.32472320797	458.892503377454
State 20	200.000000000000	9220.57468903612	472.176688779255
	300.000000000000	101.324996582814	-270.351631287198
	300.000000000000	1114.57496241096	136.388360110916
State 21	300.000000000000	2127.82492823910	245.210534489792
State 22	300.000000000000	3141.07489406725	306.461374314100
State 23	300.000000000000	4154.32485989539	347.458728047415
State 24	300.000000000000	5167.57482572354	376.884506602300
State 25	300.000000000000	6180.82479155168	398.763634236129

State 26	300.000000000000	7194.07475737983	442.605452372221
State 27	300.000000000000	8207.32472320797	485.219583620279
State 28	300.000000000000	9220.57468903612	524.076129175482
State 29	400.000000000000	101.324996582814	-269.718486252623
State 30	400.000000000000	1114.57496241096	134.489710998248
State 31	400.000000000000	2127.82492823910	237.445016110365
State 32	400.000000000000	3141.07489406725	294.284359183966
State 33	400.000000000000	4154.32485989539	362.447014846926
State 34	400.000000000000	5167.57482572354	433.664388986652
State 35	400.000000000000	6180.82479155168	495.085671565623
State 36	400.000000000000	7194.07475737983	549.345941065343
State 37	400.000000000000	8207.32472320797	598.111771383037
State 38	400.000000000000	9220.57468903612	642.555043493401
State 39	500.000000000000	101.324996582814	-270.323948216264
State 40	500.000000000000	1114.57496241096	131.442293745144
State 41	500.000000000000	2127.82492823910	233.796916027830
State 42	500.000000000000	3141.07489406725	358.152570021077
State 43	500.000000000000	4154.32485989539	455.430832284024
State 44	500.000000000000	5167.57482572354	536.199430337014
State 45	500.000000000000	6180.82479155168	605.735753501660
State 46	500.000000000000	7194.07475737983	667.085393201474
State 47	500.000000000000	8207.32472320797	722.175203662504
State 48	500.000000000000	9220.57468903612	772.310933147777
State 49	600.000000000000	101.324996582814	-271.826596717478
State 50	600.000000000000	1114.57496241096	128.762802591931
State 51	600.000000000000	2127.82492823910	309.286351764295
State 52	600.000000000000	3141.07489406725	450.224306111122
State 53	600.000000000000	4154.32485989539	560.206784937287
State 54	600.000000000000	5167.57482572354	651.387733898839
State 55	600.000000000000	6180.82479155168	729.794891265848
State 56	600.000000000000	7194.07475737983	798.912797658910
State 57	600.000000000000	8207.32472320797	860.934194241156
State 58	600.000000000000	9220.57468903612	917.348829145201
State 59	700.000000000000	101.324996582814	-274.082498916798
State 60	700.000000000000	1114.57496241096	161.317431055360
State 61	700.000000000000	2127.82492823910	392.461851977521
State 62	700.000000000000	3141.07489406725	543.423621996282
State 63	700.000000000000	4154.32485989539	656.795421021006
State 64	700.000000000000	5167.57482572354	751.300645105275
State 65	700.000000000000	6180.82479155168	832.882038749527
State 66	700.000000000000	7194.07475737983	904.996268661316

State 67	700.000000000000	8207.32472320797	969.844652166077
State 68	700.000000000000	9220.57468903612	1028.92241598606
State 69	800.000000000000	101.324996582814	-277.650510353331
State 70	800.000000000000	1114.57496241096	215.024506105903
State 71	800.000000000000	2127.82492823910	441.187170707552
State 72	800.000000000000	3141.07489406725	600.732795271870
State 73	800.000000000000	4154.32485989539	726.477313267147
State 74	800.000000000000	5167.57482572354	831.372875119556
State 75	800.000000000000	6180.82479155168	921.975850257713
State 76	800.000000000000	7194.07475737983	1002.10019112508
State 77	800.000000000000	8207.32472320797	1074.17856496743
State 78	800.000000000000	9220.57468903612	1139.86268001659
State 79	900.000000000000	101.324996582814	-279.167683128955
State 80	900.000000000000	1114.57496241096	233.574114806703
State 81	900.000000000000	2127.82492823910	479.304025330868
State 82	900.000000000000	3141.07489406725	652.677804036213
State 83	900.000000000000	4154.32485989539	789.341427193571
State 84	900.000000000000	5167.57482572354	903.360822160295
State 85	900.000000000000	6180.82479155168	1001.85516818816
State 86	900.000000000000	7194.07475737983	1088.96658576115
State 87	900.000000000000	8207.32472320797	1167.33532396393
State 88	900.000000000000	9220.57468903612	1238.75510127812
State 89	1000.00000000000	101.324996582814	-278.117525627929
State 90	1000.00000000000	1114.57496241096	250.890527060581
State 91	1000.00000000000	2127.82492823910	513.932822817271
State 92	1000.00000000000	3141.07489406725	699.186553515034
State 93	1000.00000000000	4154.32485989539	845.074387171873
State 94	1000.00000000000	5167.57482572354	966.719053855935
State 95	1000.00000000000	6180.82479155168	1071.74665627001
State 96	1000.00000000000	7194.07475737983	1164.60604066936
State 97	1000.00000000000	8207.32472320797	1248.11671741204
State 98	1000.00000000000	9220.57468903612	1324.20109147738
State 99	1100.00000000000	101.324996582814	-276.156179192518
State 100	1100.00000000000	1114.57496241096	267.923144592580
State 101	1100.00000000000	2127.82492823910	547.594024173801
State 102	1100.00000000000	3141.07489406725	744.121838119367
State 103	1100.00000000000	4154.32485989539	898.709759547733
State 104	1100.00000000000	5167.57482572354	1027.50389973744
State 105	1100.00000000000	6180.82479155168	1138.64445052746
State 106	1100.00000000000	7194.07475737983	1236.85711773708
State 107	1100.00000000000	8207.32472320797	1325.15443650220

State 108	1100.00000000000	9220.57468903612	1405.55993214460
State 109	1200.00000000000	101.324996582814	-273.806887854284
State 110	1200.00000000000	1114.57496241096	284.919693993943
State 111	1200.00000000000	2127.82492823910	581.022032779270
State 112	1200.00000000000	3141.07489406725	788.644559542336
State 113	1200.00000000000	4154.32485989539	951.774844956393
State 114	1200.00000000000	5167.57482572354	1087.58310986435
State 115	1200.00000000000	6180.82479155168	1204.71023106165
State 116	1200.00000000000	7194.07475737983	1308.16472434432
State 117	1200.00000000000	8207.32472320797	1401.12583674835
State 118	1200.00000000000	9220.57468903612	1485.76080868156
State 119	1300.00000000000	101.324996582814	-271.167660872410
State 120	1300.00000000000	1114.57496241096	301.943710551679
State 121	1300.00000000000	2127.82492823910	614.400128151065
State 122	1300.00000000000	3141.07489406725	833.040582317062
State 123	1300.00000000000	4154.32485989539	1004.64860892806
State 124	1300.00000000000	5167.57482572354	1147.40448592089
State 125	1300.00000000000	6180.82479155168	1270.45414327325
State 126	1300.00000000000	7194.07475737983	1379.08606206339
State 127	1300.00000000000	8207.32472320797	1476.66038485591
State 128	1300.00000000000	9220.57468903612	1565.45671629202
State 129	1400.00000000000	101.324996582814	-268.252093483698
State 130	1400.00000000000	1114.57496241096	319.055285167224
State 131	1400.00000000000	2127.82492823910	647.870501435276
State 132	1400.00000000000	3141.07489406725	877.514614695943
State 133	1400.00000000000	4154.32485989539	1057.57171756820
State 134	1400.00000000000	5167.57482572354	1207.24886994026
State 135	1400.00000000000	6180.82479155168	1336.18925148511
State 136	1400.00000000000	7194.07475737983	1449.95936691771
State 137	1400.00000000000	8207.32472320797	1552.10397748274
State 138	1400.00000000000	9220.57468903612	1645.01598503573
State 139	1500.00000000000	101.324996582814	-265.045282841618
State 140	1500.00000000000	1114.57496241096	336.344095689079
State 141	1500.00000000000	2127.82492823910	681.627888309691
State 142	1500.00000000000	3141.07489406725	922.324348664146
State 143	1500.00000000000	4154.32485989539	1110.85027502381
State 144	1500.00000000000	5167.57482572354	1267.45368641414
State 145	1500.00000000000	6180.82479155168	1402.27374939524
State 146	1500.00000000000	7194.07475737983	1521.16552301108
State 147	1500.00000000000	8207.32472320797	1627.84628430693
State 148	1500.00000000000	9220.57468903612	1724.84403890126

State 149	1600.00000000000	101.324996582814	-296.191746748731
State 150	1600.00000000000	1114.57496241096	353.941248001353
State 151	1600.00000000000	2127.82492823910	715.923858821046
State 152	1600.00000000000	3141.07489406725	967.800379917955
State 153	1600.00000000000	4154.32485989539	1164.87684338060
State 154	1600.00000000000	5167.57482572354	1328.44868816481
State 155	1600.00000000000	6180.82479155168	1469.16558307408
State 156	1600.00000000000	7194.07475737983	1593.17843544973
State 157	1600.00000000000	8207.32472320797	1704.39006592395
State 158	1600.00000000000	9220.57468903612	1805.44270317966
State 159	1700.00000000000	101.324996582814	-356.690346632737
State 160	1700.00000000000	1114.57496241096	372.019677476788
State 161	1700.00000000000	2127.82492823910	751.089659069867
State 162	1700.00000000000	3141.07489406725	1014.38074884431
State 163	1700.00000000000	4154.32485989539	1220.14638189667
State 164	1700.00000000000	5167.57482572354	1390.77265878996
State 165	1700.00000000000	6180.82479155168	1537.43784099923
State 166	1700.00000000000	7194.07475737983	1666.59694197492
State 167	1700.00000000000	8207.32472320797	1782.34406819852
State 168	1700.00000000000	9220.57468903612	1887.44819035001
State 169	1800.00000000000	101.324996582814	-432.117723548778
State 170	1800.00000000000	1114.57496241096	390.800730229048
State 171	1800.00000000000	2127.82492823910	787.562454380455
State 172	1800.00000000000	3141.07489406725	1062.59463148466
State 173	1800.00000000000	4154.32485989539	1277.26386671080
State 174	1800.00000000000	5167.57482572354	1455.08389035601
State 175	1800.00000000000	6180.82479155168	1607.78797016691
State 176	1800.00000000000	7194.07475737983	1742.15085723586
State 177	1800.00000000000	8207.32472320797	1862.46582302839
State 178	1800.00000000000	9220.57468903612	1971.63666025623
State 179	1900.00000000000	101.324996582814	-461.304101471256
State 180	1900.00000000000	1114.57496241096	410.560948748285
State 181	1900.00000000000	2127.82492823910	825.834044321478
State 182	1900.00000000000	3141.07489406725	1113.08316147660
State 183	1900.00000000000	4154.32485989539	1336.95474949796
State 184	1900.00000000000	5167.57482572354	1522.16850933427
State 185	1900.00000000000	6180.82479155168	1681.04830602152
State 186	1900.00000000000	7194.07475737983	1820.71184053284
State 187	1900.00000000000	8207.32472320797	1945.66068949615
State 188	1900.00000000000	9220.57468903612	2058.94405179146
State 189	2000.00000000000	101.324996582814	-492.983469868330

State 190	2000.00000000000	1114.57496241096	431.636510850525
State 191	2000.00000000000	2127.82492823910	866.518665093150
State 192	2000.00000000000	3141.07489406725	1166.59979314921
State 193	2000.00000000000	4154.32485989539	1400.06720943001
State 194	2000.00000000000	5167.57482572354	1592.94423736201
State 195	2000.00000000000	6180.82479155168	1758.19088006740
State 196	2000.00000000000	7194.07475737983	1903.29230723831
State 197	2000.00000000000	8207.32472320797	2032.97392473578
State 198	2000.00000000000	9220.57468903612	2150.45310790350
State 199	2000.00000000000	9220.57468903612	2150.45310790350
State 200	2000.00000000000	9220.57468903612	2150.45310790350

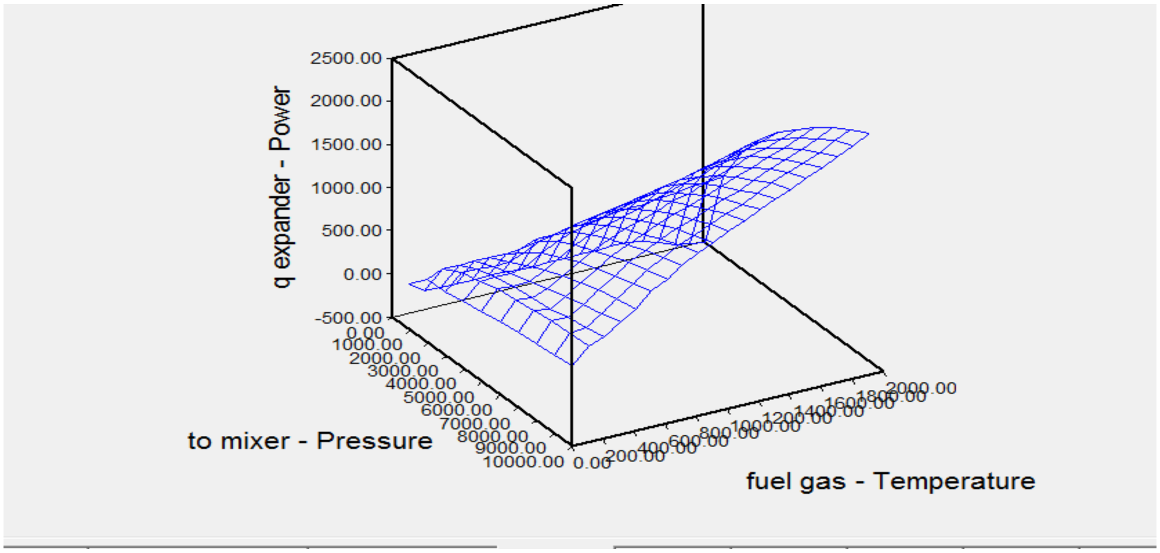


Fig. 5.32: Surface plot showing effect of fuel gas temperature, mixer pressure on Power Produced

Conclusions

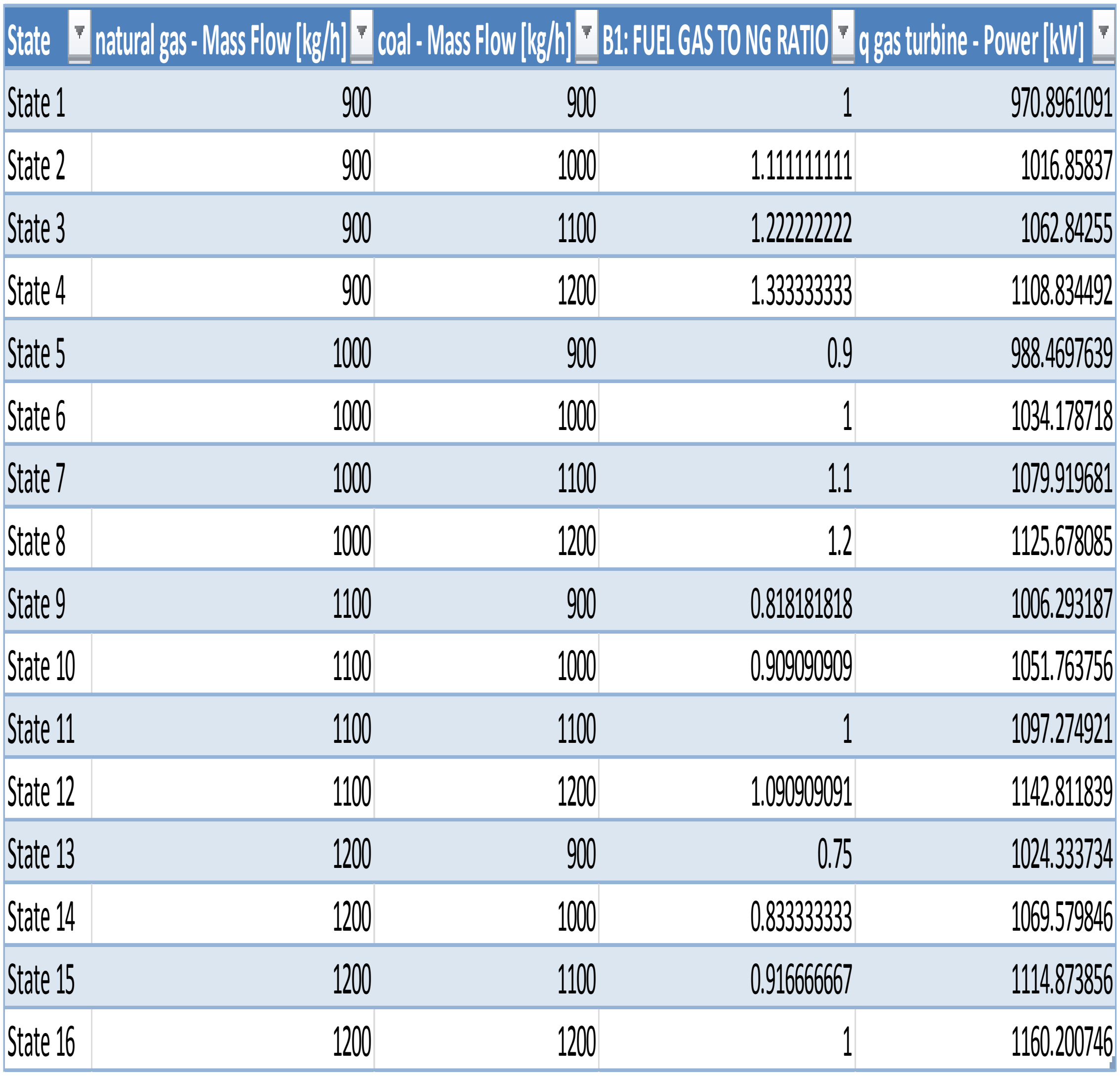
- The fuel gas temperature and pressure of feed to the gas turbine are in direct proportion with the power produced in gas turbine.
- As fuel gas temperature and to mixer pressure increases, the power produced increases.
- Optimum value of temperature of fuel gas is taken as 900 to 1500 ^{o}C.

5.9.4 Case 4: The effect of coal to natural gas flow rate on power produced is studied.

- We first calculated the ratio of coal mass flow rate to natural gas mass flow rate and then its effect on power produced is analyzed
- Independent variable- coal mass flow rate and natural gas mass flow rate
- Dependent variable - power produced in gas turbine.

Table 5.6 provides the Optimization data developed whereas figure 5.33 shows the analysis for effect of coal and natural gas flowrate on power production.

Table 5.6: Optimization data for coal mass flow rate and natural gas mass flow rate and its effect on power produced in gas turbine



State	natural gas - Mass Flow [kg/h]	coal - Mass Flow [kg/h]	B1: FUEL GAS TO NG RATIO	q gas turbine - Power [kW]
State 1	900	900	1	970.8961091
State 2	900	1000	1.111111111	1016.85837
State 3	900	1100	1.222222222	1062.84255
State 4	900	1200	1.333333333	1108.834492
State 5	1000	900	0.9	988.4697639
State 6	1000	1000	1	1034.178718
State 7	1000	1100	1.1	1079.919681
State 8	1000	1200	1.2	1125.678085
State 9	1100	900	0.818181818	1006.293187
State 10	1100	1000	0.909090909	1051.763756
State 11	1100	1100	1	1097.274921
State 12	1100	1200	1.090909091	1142.811839
State 13	1200	900	0.75	1024.333734
State 14	1200	1000	0.833333333	1069.579846
State 15	1200	1100	0.916666667	1114.873856
State 16	1200	1200	1	1160.200746

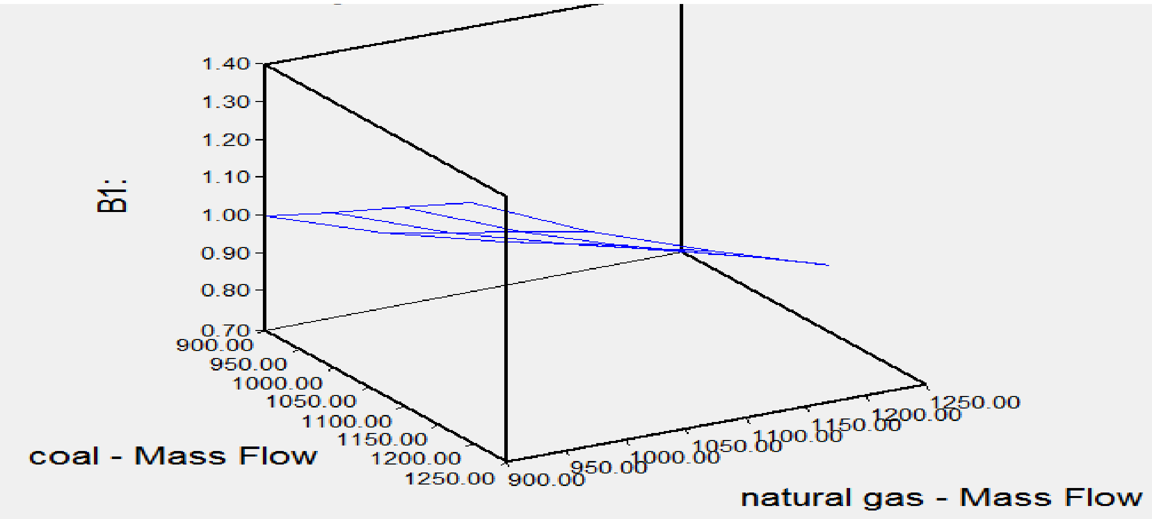


Fig. 5.33: Plot for coal mass flow rate and natural gas mass flow rate and its effect on power produced in gas turbine

Conclusions

The ratio of coal and natural gas flow rates vs power produced graph shows that;

- As the ratio increases power generated increases
- As natural gas flow rate increases the power generated increases

5.9.5 Case 5: Effect of fuel gas and natural gas flow rate on power produced is analyzed.

- The fuel gas is produced from the gasification of coal in presence of steam and oxygen. The flow rate of fuel gas is the sum of flow rates of coal, steam, and oxygen.
- Ratio of flow rates of fuel gas and natural gas is compared with the power produced in the gas turbine.

Table 5.7 provides the data for ratio of fuel gas and natural gas mass flowrate on Power.

Conclusion: From the table, it is seen that, as fuel and natural gas flowrates rise, the power production rises. But it depends on the capacity needed. Also, the auxiliary power also rises. Hence, requirement of power is the only parameter to choose.

Table 5.7: Data for effect of ratio of fuel gas and natural gas mass flowrate on power

State	coal - Mass Flow...	oxygen - Mass F...	Natural Gas - Ma...	steam - Mass Fl...	Q steam comp - ...	q compressor (o...	q fuel gas comp -...	Power Gas Turbi...	q ng comp - Pow...
State 1	1000	1000	1000	1000	453.9	346.6	173.2	1413	415.3
State 2	1000	1000	1000	3000	1362	346.6	312.1	2382	415.3
State 3	1000	1000	1000	5000	2270	346.6	450.8	3351	415.3
State 4	1000	1000	3000	1000	453.9	346.6	173.2	1940	1246
State 5	1000	1000	3000	3000	1362	346.6	312.1	2888	1246
State 6	1000	1000	3000	5000	2270	346.6	450.8	3840	1246
State 7	1000	1000	5000	1000	453.9	346.6	173.2	2486	2077
State 8	1000	1000	5000	3000	1362	346.6	312.1	3422	2077
State 9	1000	1000	5000	5000	2270	346.6	450.8	4362	2077
State 10	1000	3000	1000	1000	453.9	1040	212.9	1752	415.3
State 11	1000	3000	1000	3000	1362	1040	351.7	2712	415.3
State 12	1000	3000	1000	5000	2270	1040	490.4	3677	415.3
State 13	1000	3000	3000	1000	453.9	1040	212.9	2280	1246
State 14	1000	3000	3000	3000	1362	1040	351.7	3218	1246
State 15	1000	3000	3000	5000	2270	1040	490.4	4166	1246
State 16	1000	3000	5000	1000	453.9	1040	212.9	2827	2077
State 17	1000	3000	5000	3000	1362	1040	351.7	3752	2077
State 18	1000	3000	5000	5000	2270	1040	490.4	4688	2077
State 19	1000	5000	1000	1000	453.9	1733	291.9	2259	415.3
State 20	1000	5000	1000	3000	1362	1733	430.7	3223	415.3
State 21	1000	5000	1000	5000	2270	1733	569.5	4190	415.3
State 22	1000	5000	3000	1000	453.9	1733	291.9	2770	1246
State 23	1000	5000	3000	3000	1362	1733	430.7	3716	1246
State 24	1000	5000	3000	5000	2270	1733	569.5	4669	1246
State 25	1000	5000	5000	1000	453.9	1733	291.9	3308	2077
State 26	1000	5000	5000	3000	1362	1733	430.7	4241	2077
State 27	1000	5000	5000	5000	2270	1733	569.5	5183	2077
State 28	3000	1000	1000	1000	453.9	346.6	359.8	2509	415.3
State 29	3000	1000	1000	3000	1362	346.6	521.0	3600	415.3
State 30	3000	1000	1000	5000	2270	346.6	660.5	4595	415.3
State 31	3000	1000	3000	1000	453.9	346.6	359.8	2998	1246
State 32	3000	1000	3000	3000	1362	346.6	521.0	4070	1246
State 33	3000	1000	3000	5000	2270	346.6	660.5	5053	1246
State 34	3000	1000	5000	1000	453.9	346.6	359.8	3522	2077
State 35	3000	1000	5000	3000	1362	346.6	521.0	4579	2077
State 36	3000	1000	5000	5000	2270	346.6	660.5	5552	2077
State 37	3000	3000	1000	1000	453.9	1040	380.9	2774	415.3
State 38	3000	3000	1000	3000	1362	1040	519.7	3760	415.3
State 39	3000	3000	1000	5000	2270	1040	658.6	4740	415.3
State 40	3000	3000	3000	1000	453.9	1040	380.9	3265	1246
State 41	3000	3000	3000	3000	1362	1040	519.7	4238	1246
State 42	3000	3000	3000	5000	2270	1040	658.6	5207	1246
State 43	3000	3000	5000	1000	453.9	1040	380.9	3791	2077
State 44	3000	3000	5000	3000	1362	1040	519.7	4752	2077
State 45	3000	3000	5000	5000	2270	1040	658.6	5712	2077
State 46	3000	5000	1000	1000	453.9	1733	378.8	2939	415.3
State 47	3000	5000	1000	3000	1362	1733	517.5	3909	415.3
State 48	3000	5000	1000	5000	2270	1733	656.3	4880	415.3
State 49	3000	5000	3000	1000	453.9	1733	378.8	3447	1246
State 50	3000	5000	3000	3000	1362	1733	517.5	4401	1246
State 51	3000	5000	3000	5000	2270	1733	656.3	5359	1246
State 52	3000	5000	5000	1000	453.9	1733	378.8	3983	2077
State 53	3000	5000	5000	3000	1362	1733	517.5	4924	2077
State 54	3000	5000	5000	5000	2270	1733	656.3	5872	2077
State 55	5000	1000	1000	1000	453.9	346.6	368.5	2877	415.3
State 56	5000	1000	1000	3000	1362	346.6	715.8	4744	415.3
State 57	5000	1000	1000	5000	2270	346.6	867.7	5801	415.3
State 58	5000	1000	3000	1000	453.9	346.6	368.5	3384	1246
State 59	5000	1000	3000	3000	1362	346.6	715.8	5193	1246
State 60	5000	1000	3000	5000	2270	346.6	867.7	6241	1246
State 61	5000	1000	5000	1000	453.9	346.6	368.5	3918	2077
State 62	5000	1000	5000	3000	1362	346.6	715.8	5684	2077
State 63	5000	1000	5000	5000	2270	346.6	867.7	6722	2077
State 64	5000	3000	1000	1000	453.9	1040	586.7	3949	415.3
State 65	5000	3000	1000	3000	1362	1040	728.7	4971	415.3
State 66	5000	3000	1000	5000	2270	1040	868.1	5969	415.3
State 67	5000	3000	3000	1000	453.9	1040	586.7	4410	1246
State 68	5000	3000	3000	3000	1362	1040	728.7	5421	1246
State 69	5000	3000	3000	5000	2270	1040	868.1	6413	1246
State 70	5000	3000	5000	1000	453.9	1040	586.7	4912	2077
State 71	5000	3000	5000	3000	1362	1040	728.7	5914	2077
State 72	5000	3000	5000	5000	2270	1040	868.1	6897	2077
State 73	5000	5000	1000	1000	453.9	1733	588.5	4143	415.3
State 74	5000	5000	1000	3000	1362	1733	727.4	5136	415.3
State 75	5000	5000	1000	5000	2270	1733	866.2	6122	415.3
State 76	5000	5000	3000	1000	453.9	1733	588.5	4610	1246
State 77	5000	5000	3000	3000	1362	1733	727.4	5594	1246
State 78	5000	5000	3000	5000	2270	1733	866.2	6574	1246
State 79	5000	5000	5000	1000	453.9	1733	588.5	5116	2077
State 80	5000	5000	5000	3000	1362	1733	727.4	6092	2077
State 81	5000	5000	5000	5000	2270	1733	866.2	7063	2077

5.9.6 Case 6: Effect of inlet feed pressure on net power generated is analyzed. In this case we are comparing the effect of inlet feed pressure on power.

Independent variables:

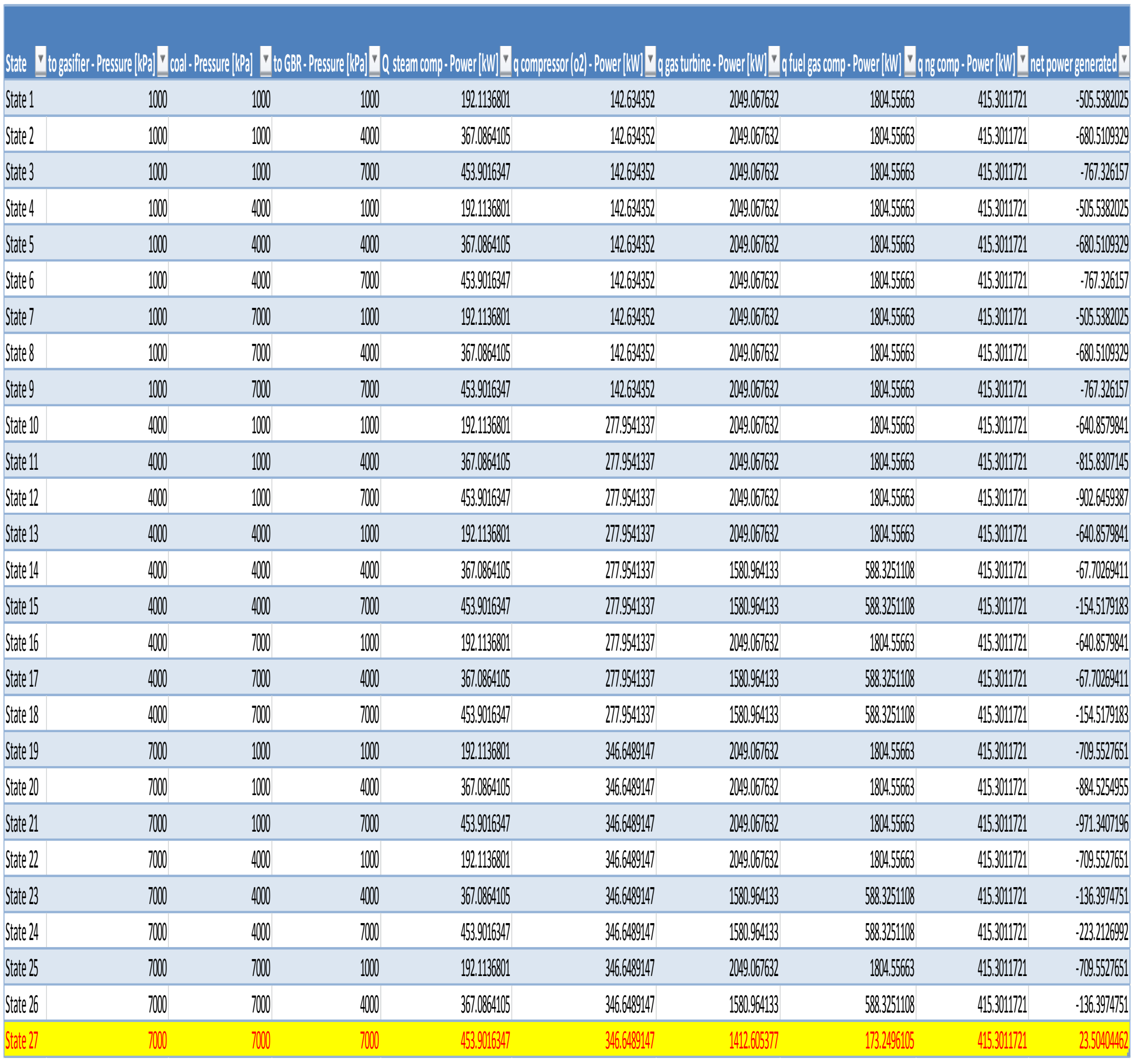
- Feed inlet pressures

Dependent variables:

- Feed compression power
- Natural gas compression power
- Fuel gas compression power
- Gas turbine power generated

Table 5.8 provides the necessary data generated.

Table 5.8: Data for optimization analysis of effect of inlet feed pressure on power



State	to gasifier - Pressure [kPa]	coal - Pressure [kPa]	to GBR - Pressure [kPa]	Q steam comp - Power [kW]	q compressor (o2) - Power [kW]	q gas turbine - Power [kW]	q fuel gas comp - Power [kW]	q ng comp - Power [kW]	net power generated
State 1	1000	1000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 2	1000	1000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 3	1000	1000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 4	1000	4000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 5	1000	4000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 6	1000	4000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 7	1000	7000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 8	1000	7000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 9	1000	7000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 10	4000	1000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 11	4000	1000	4000	367.0864105	277.9541337	2049.067632	1804.55663	415.3011721	-815.8307145
State 12	4000	1000	7000	453.9016347	277.9541337	2049.067632	1804.55663	415.3011721	-902.6459387
State 13	4000	4000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 14	4000	4000	4000	367.0864105	277.9541337	1580.964133	588.3251108	415.3011721	-67.70269411
State 15	4000	4000	7000	453.9016347	277.9541337	1580.964133	588.3251108	415.3011721	-154.5179183
State 16	4000	7000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 17	4000	7000	4000	367.0864105	277.9541337	1580.964133	588.3251108	415.3011721	-67.70269411
State 18	4000	7000	7000	453.9016347	277.9541337	1580.964133	588.3251108	415.3011721	-154.5179183
State 19	7000	1000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 20	7000	1000	4000	367.0864105	346.6489147	2049.067632	1804.55663	415.3011721	-884.5254955
State 21	7000	1000	7000	453.9016347	346.6489147	2049.067632	1804.55663	415.3011721	-971.3407196
State 22	7000	4000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 23	7000	4000	4000	367.0864105	346.6489147	1580.964133	588.3251108	415.3011721	-136.3974751
State 24	7000	4000	7000	453.9016347	346.6489147	1580.964133	588.3251108	415.3011721	-223.2126992
State 25	7000	7000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 26	7000	7000	4000	367.0864105	346.6489147	1580.964133	588.3251108	415.3011721	-136.3974751
State 27	7000	7000	7000	453.9016347	346.6489147	1412.605377	173.2496105	415.3011721	23.50404462

Conclusions

- The overall power generated is calculated for different combinations of feed pressures.
- Net power generated=(power generated in gas turbine+ steam turbine)-(power consumed in compression of feeds)
- From calculation in excel spreadsheet, it can be inferred that for stage 27, process details are:
  - ❖ Feed to gasifier pressure = 7000 kPa
  - ❖ Feed to gas turbine pressure= 9000 kPa
  - ❖ Net power generated is 23. 5 kW

So this is the optimum condition to be used while operating the power plant.

5.9.7 Case 7: Effect of oxygen flow rate on power produced in the gas turbine is studied.

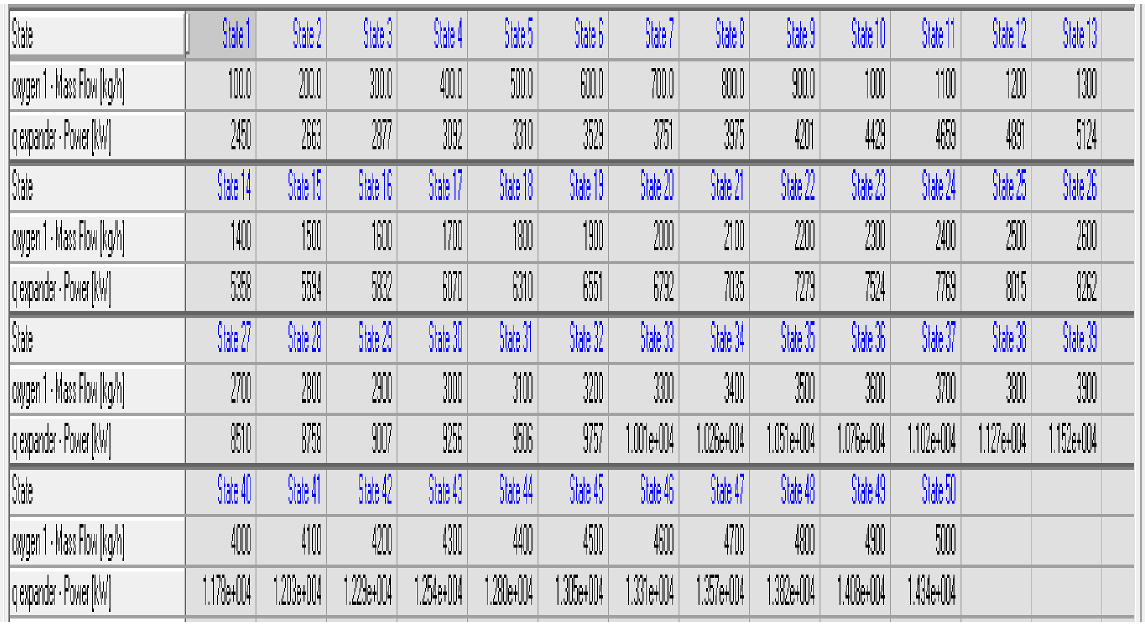
The variable chosen for the optimization study are:

Independent variable: oxygen flow rate (kg/hr)

Dependent variable: power produced in gas turbine

Table 5.9 provides the calculation details and figure 5.34 provides the results.

Table 5.9: Effect of Oxygen flow rate on power produced in the gas turbine.



State	State 1	State 2	State 3	State 4	State 5	State 6	State 7	State 8	State 9	State 10	State 11	State 12	State 13
oxygen 1 - Mass Flow [kg/h]	100.0	200.0	300.0	400.0	500.0	600.0	700.0	800.0	900.0	1000	1100	1200	1300
q expander - Power [kW]	2450	2663	2877	3092	3310	3529	3751	3975	4201	4429	4659	4891	5124

State	State 14	State 15	State 16	State 17	State 18	State 19	State 20	State 21	State 22	State 23	State 24	State 25	State 26
oxygen 1 - Mass Flow [kg/h]	1400	1500	1600	1700	1800	1900	2000	2100	2200	2300	2400	2500	2600
q expander - Power [kW]	5358	5594	5832	6070	6310	6551	6792	7035	7279	7524	7769	8015	8262

State	State 27	State 28	State 29	State 30	State 31	State 32	State 33	State 34	State 35	State 36	State 37	State 38	State 39
oxygen 1 - Mass Flow [kg/h]	2700	2800	2900	3000	3100	3200	3300	3400	3500	3600	3700	3800	3900
q expander - Power [kW]	8510	8758	9007	9256	9506	9757	1.001e+004	1.026e+004	1.051e+004	1.076e+004	1.102e+004	1.127e+004	1.152e+004

State	State 40	State 41	State 42	State 43	State 44	State 45	State 46	State 47	State 48	State 49	State 50		
oxygen 1 - Mass Flow [kg/h]	4000	4100	4200	4300	4400	4500	4600	4700	4800	4900	5000		
q expander - Power [kW]	1.178e+004	1.203e+004	1.229e+004	1.254e+004	1.280e+004	1.305e+004	1.331e+004	1.357e+004	1.382e+004	1.408e+004	1.434e+004		

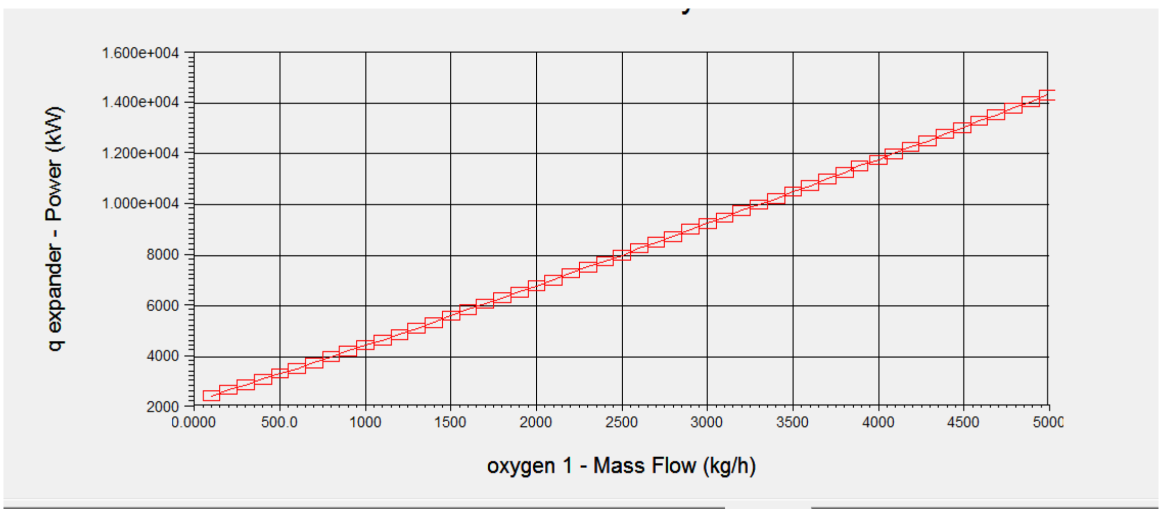


Fig. 5.34: Relationship between oxygen mass flow and power generated

Conclusion

There is a linear relation between oxygen flow rate and power produced. Hence, proper oxygen supply for combustion is essential.

5.10 RESULTS AND DISCUSSION

A process optimization method has been developed and applied to study the combined feed power generation in IGCC plant. Such studies have not been attempted till now. A detailed analysis is carried out to understand the system as well as provide viable and generic solution to industry, which is facing heavy energy crunch presently. The boundary definitions and the identification of main units are basic steps for the process analysis. Thermodynamic databases, parametric models and steady state simulations are used as fundamental tools, which are appropriately combined to gain the desired advantages**.**

A specialized simulation study using Aspen HYSYS® was performed considering coal sample using its proximate and ultimate analysis and Natural gas as another fuel. The effects of various operating parameters were studied on the final power generation. Various combinations of feeds are also considered and analyzed using simulation results.

Simulation runs were carried out by varying different parameters like feed inlet pressure, flowrates, pressure drop across gas turbine, and H_2/CO ratio.

From the optimization study carried out earlier, following observations are made:

5.10.1 Temperature of fuel gas

Figure 5.35 shows the effect of fuel gas temperature on power. The graph shows that the power produced increases with the temperature of the fuel gas. From this study, we can conclude the optimum temperature lies between 1200 to 1300 ^{o}C.

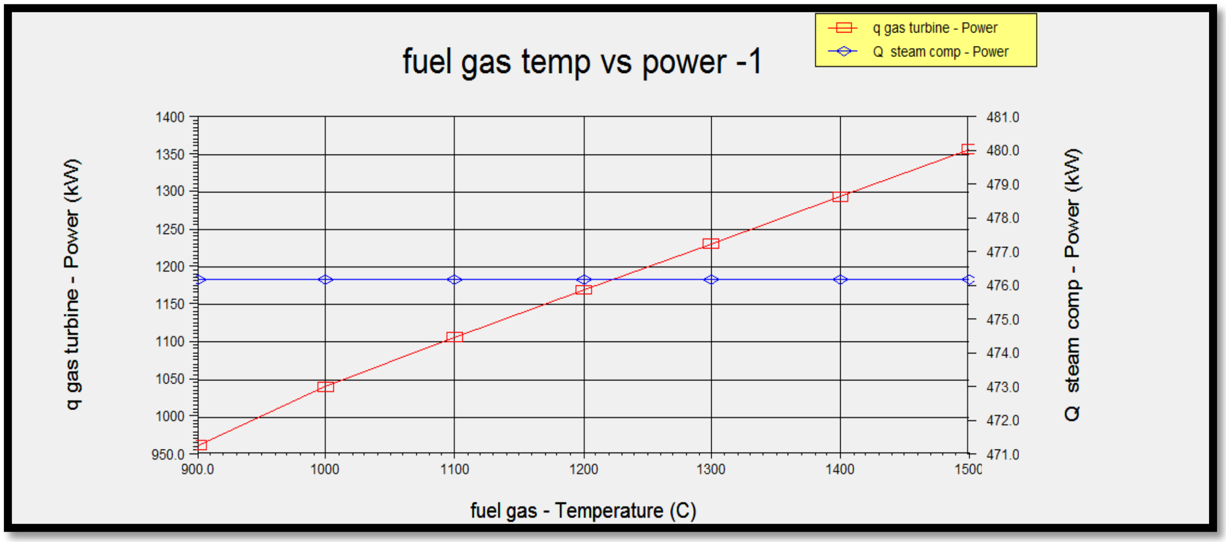


Fig. 5.35: Effect of fuel gas temperature on power

5.10.2 H_2 to CO ratio

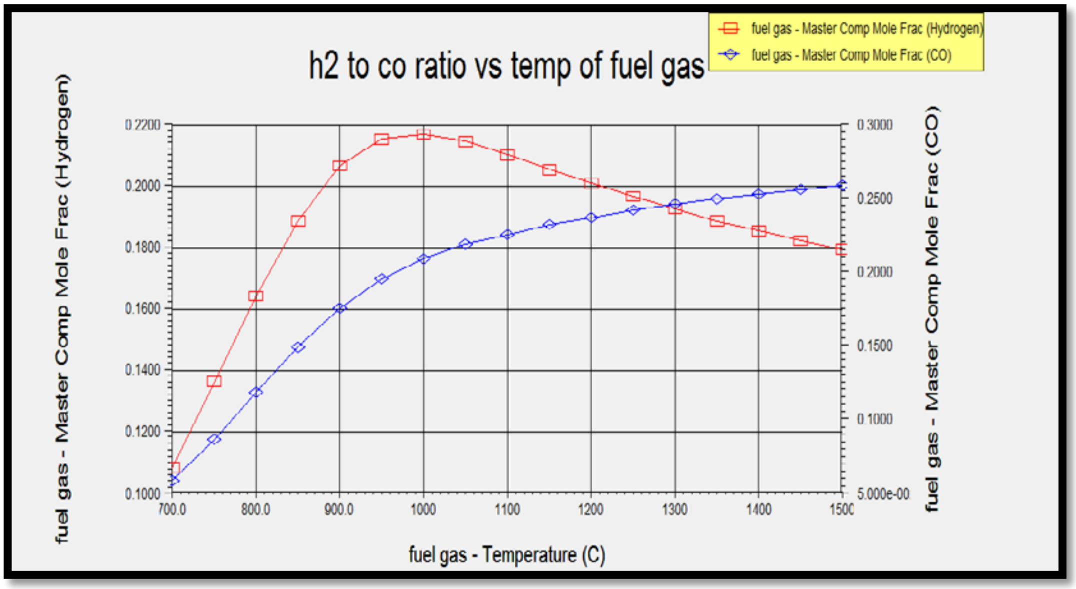


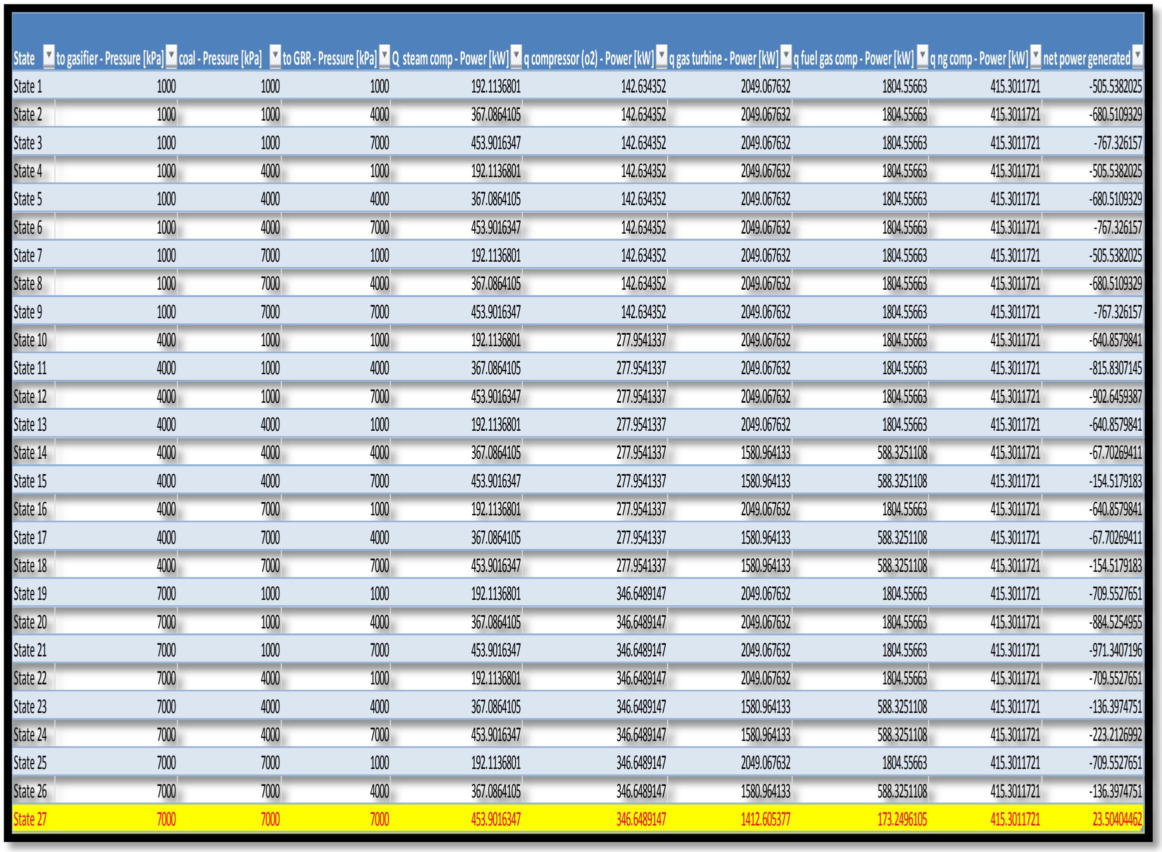
Fig. 5.36: Effect of fuel gas temperature on H_2 / CO ratio

From the figure 5.36, it is seen that the H_2/CO ratio increases till 1000 ^oC and then starts decreasing. So from this result, we get the optimum temperature as 1000 ^oC. While the earlier result of temperature of fuel gas suggests to work between 1200 to 1300 ^oC. Considering the two results, minor reduction in H_2/CO ratio is accepted and 1100 to 1200 ^oC is chosen as the optimum temperature for the process.

5.10.3 Effect of Feed Pressure on Power generation

Table 5.10 provides data for analysis of effect of feed pressure on power generated.

Table 5.10: Data for Feed Pressure and Power.



State	to gasifier - Pressure [kPa]	coal - Pressure [kPa]	to GBR - Pressure [kPa]	Q steam comp - Power [kW]	q compressor (o2) - Power [kW]	q gas turbine - Power [kW]	q fuel gas comp - Power [kW]	q ng comp - Power [kW]	net power generated
State 1	1000	1000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 2	1000	1000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 3	1000	1000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 4	1000	4000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 5	1000	4000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 6	1000	4000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 7	1000	7000	1000	192.1136801	142.634352	2049.067632	1804.55663	415.3011721	-505.5382025
State 8	1000	7000	4000	367.0864105	142.634352	2049.067632	1804.55663	415.3011721	-680.5109329
State 9	1000	7000	7000	453.9016347	142.634352	2049.067632	1804.55663	415.3011721	-767.326157
State 10	4000	1000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 11	4000	1000	4000	367.0864105	277.9541337	2049.067632	1804.55663	415.3011721	-815.8307145
State 12	4000	1000	7000	453.9016347	277.9541337	2049.067632	1804.55663	415.3011721	-902.6459387
State 13	4000	4000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 14	4000	4000	4000	367.0864105	277.9541337	1580.964133	588.3251108	415.3011721	-67.70269411
State 15	4000	4000	7000	453.9016347	277.9541337	1580.964133	588.3251108	415.3011721	-154.5179183
State 16	4000	7000	1000	192.1136801	277.9541337	2049.067632	1804.55663	415.3011721	-640.8579841
State 17	4000	7000	4000	367.0864105	277.9541337	1580.964133	588.3251108	415.3011721	-67.70269411
State 18	4000	7000	7000	453.9016347	277.9541337	1580.964133	588.3251108	415.3011721	-154.5179183
State 19	7000	1000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 20	7000	1000	4000	367.0864105	346.6489147	2049.067632	1804.55663	415.3011721	-884.5254955
State 21	7000	1000	7000	453.9016347	346.6489147	2049.067632	1804.55663	415.3011721	-971.3407196
State 22	7000	4000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 23	7000	4000	4000	367.0864105	346.6489147	1580.964133	588.3251108	415.3011721	-136.3974751
State 24	7000	4000	7000	453.9016347	346.6489147	1580.964133	588.3251108	415.3011721	-223.2126992
State 25	7000	7000	1000	192.1136801	346.6489147	2049.067632	1804.55663	415.3011721	-709.5527651
State 26	7000	7000	4000	367.0864105	346.6489147	1580.964133	588.3251108	415.3011721	-136.3974751
State 27	7000	7000	7000	453.9016347	346.6489147	1412.605377	173.2496105	415.3011721	23.50404462

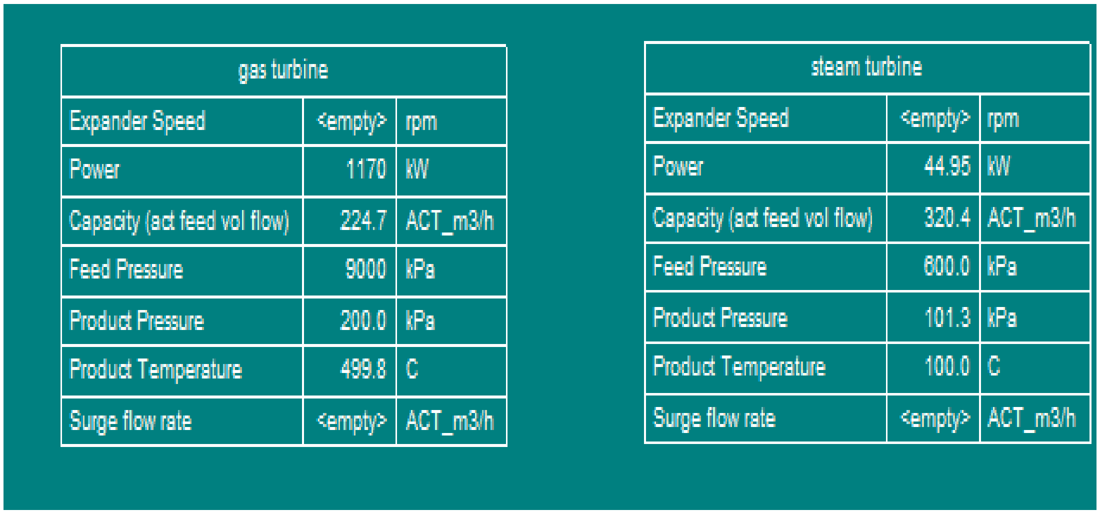
From the above table, following optimized parameters are chosen for working in the plant:

- Pressure of feed to the gasifier=7000 kPa
- Pressure of feed to gas turbine=9000 kPa

5.10.4 Power output

Total Power Produced = Power Produced from Gas turbine + Power Produced from Steam Turbine

Fig. 5.37: Gas and Steam Turbine Data



gas turbine		
Expander Speed	<empty>	rpm
Power	1170	kW
Capacity (act feed vol flow)	224.7	ACT_m3/h
Feed Pressure	9000	kPa
Product Pressure	200.0	kPa
Product Temperature	499.8	C
Surge flow rate	<empty>	ACT_m3/h

steam turbine		
Expander Speed	<empty>	rpm
Power	44.95	kW
Capacity (act feed vol flow)	320.4	ACT_m3/h
Feed Pressure	600.0	kPa
Product Pressure	101.3	kPa
Product Temperature	100.0	C
Surge flow rate	<empty>	ACT_m3/h

5.10.5 Final Power Generation

From the figure 5.37 we get,

- **For coal flow rate=1000 kg/hr**
- **Natural gas flow rate= 1000 kg/hr**

- **Total power =1214.95 kW (1170 kW from GT + 44.5 kW from ST)**
- **Total power =1.21 MW**

The power plant rated for 1 MW power generation is now producing 1.21 MW power. This is the success of the present work and outcome of the optimization study.

This capacity can be augmented to higher scale for production of 100 to 1000 to 10000 MW power plants known as Ultra Mega Power Plants (UMPPs).

Attempts to achieve similar industry scale simulations and optimization are made and reported in this thesis in chapters 1 and 6.

5.11 COMPARISON OF VARIOUS COMBINED FEED IGCC POWER PLANTS

Table 5.11 shows the achievement of the present study. All possible combinations are worked out using simulations. As simulating complete power plant is a quite big task, base case designs were performed which were scaled-up for the desired design case.

One promising option of coal and natural gas fuels has been optimized to all possible levels with all key parameters. Some highlights of the results of the present study are shown below in table 5.11.

Table 5.11: Comparative of four combined feed options worked out in the present study

Parameters	1	2	3	4
	Coal	**Coal and Biomass**	**Coal and Naphtha**	**Coal and Natural Gas**
Flow rate (kg/hr)	**1000.0**	**2000.0**	**2000.0**	**2000.0**
Feed Pressure (kPa)	**7000.0**	**7000.0**	**7000.0**	**7000.0**
Gas Turbine input Pressure (kPa)	**9000.0**	**9000.0**	**9000.0**	**9000.0**
Power Production (Gas Turbine) (kW)	**992.0**	**3112.0**	**7063.0**	**1170.0**
Power Production (Steam Turbine) (kW)	**44.95**	**44.95**	**44.95**	**44.95**
Total Compression Power Required (kW)	**973.7**	**2836.08**	**6786**	**906.73**
Total Power Produced, kW	**1037**	**3157**	**7108**	**1215**
Net Power Produced, MW	**1.037**	**3.157**	**7.108**	**1.215**

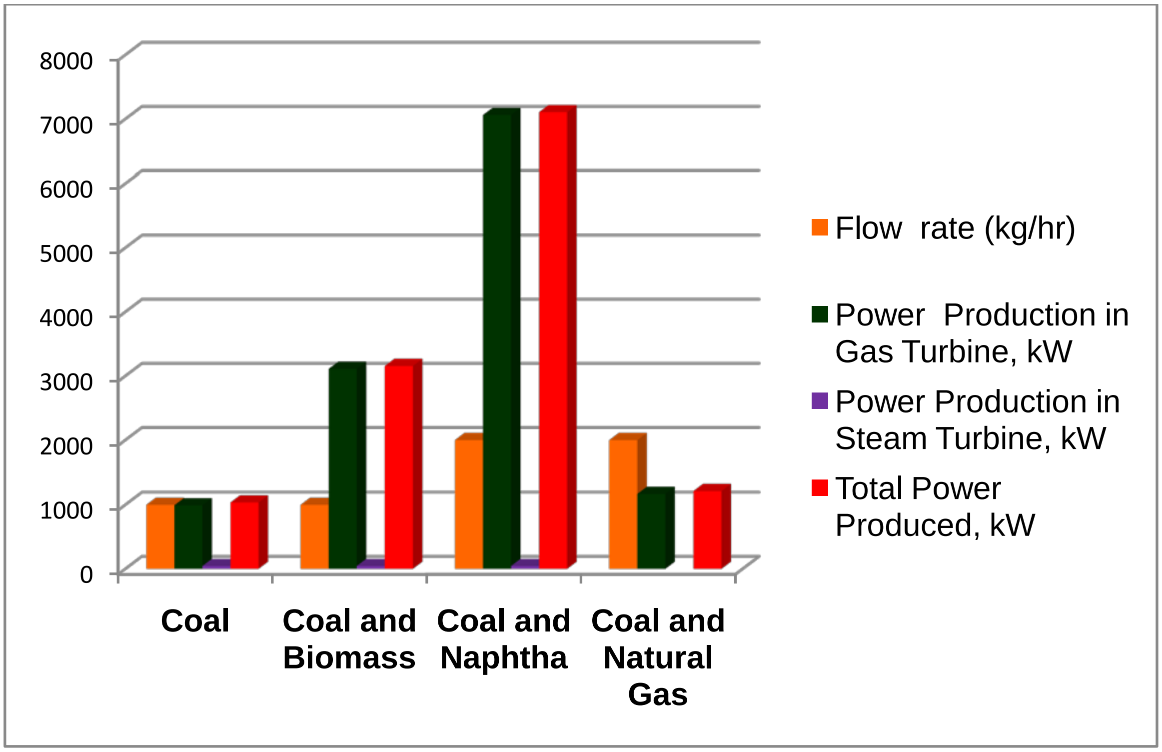


Fig. 5.38: Graphical representation of the final results

With promising results from the present study, we decided to use the similar methodology for biomass gasification and use this biomass generated synthesis gas directly in gas turbines of power plant for electricity production.

This is worked out in the next chapter i.e. chapter 6.

5.11.1 FINAL FLOW SHEETS SIMULATED IN Aspen HYSYS®

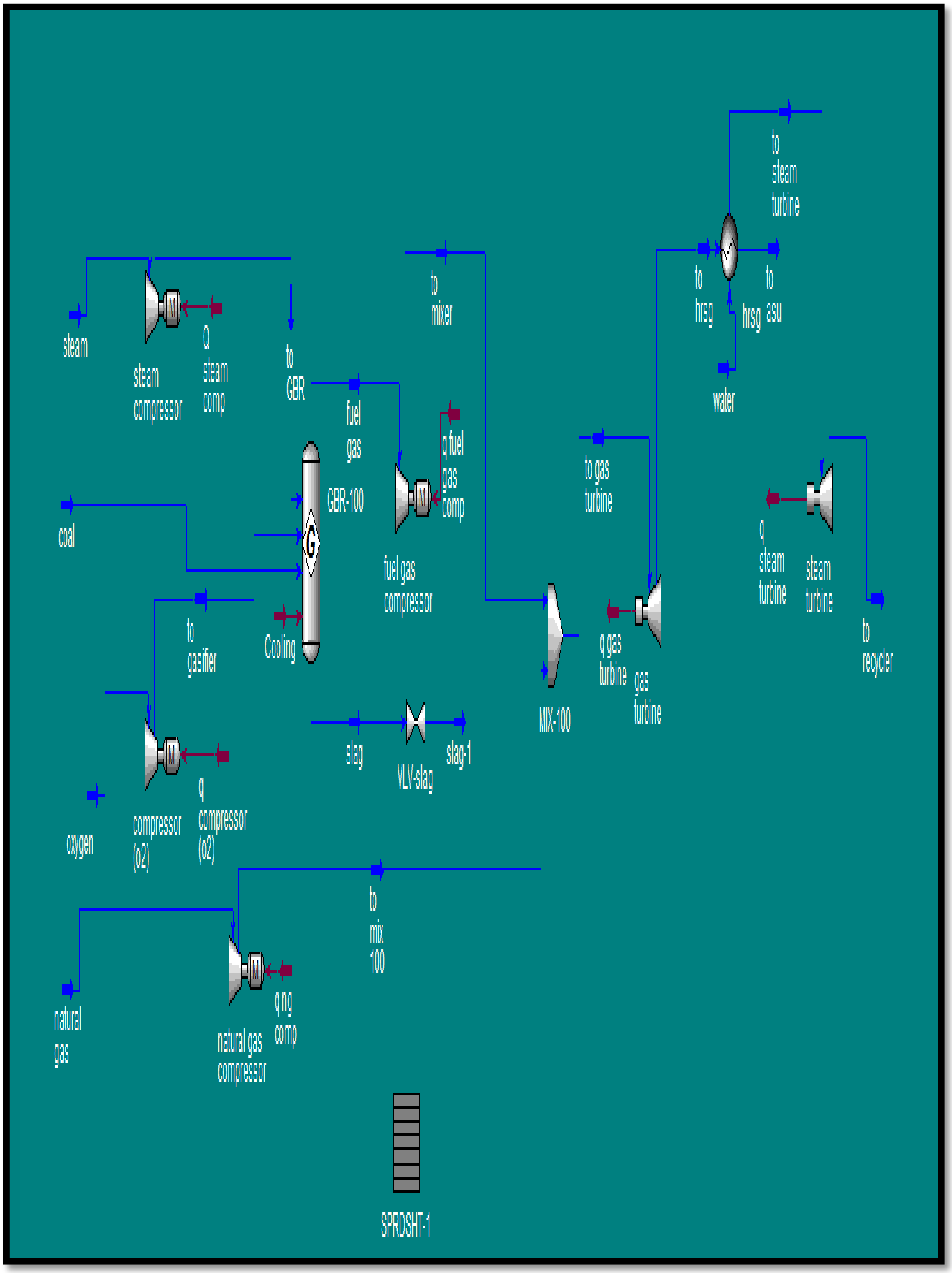
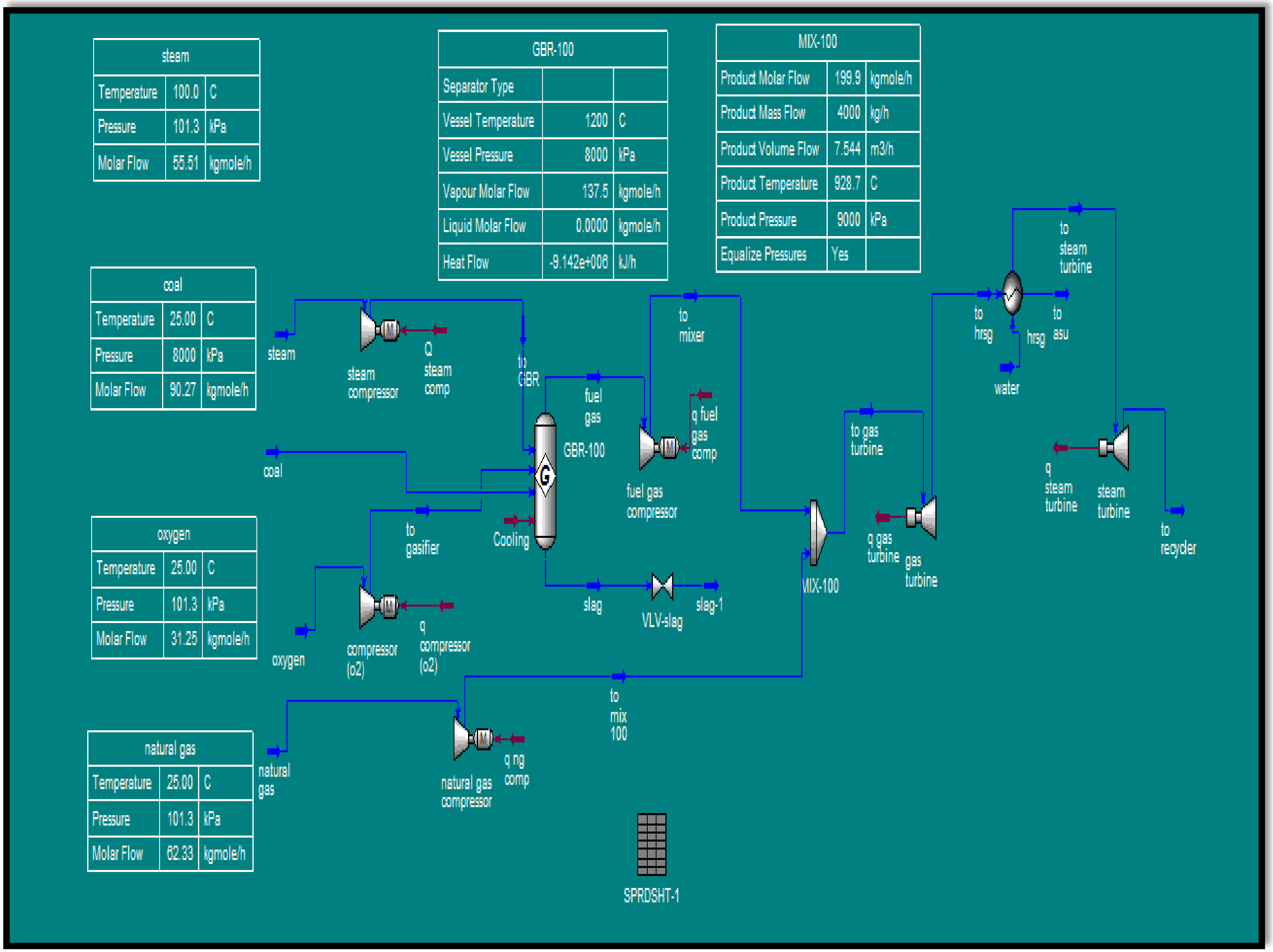


Fig. 5.39: Optimized PFD of Combined feed IGCC



steam		
Temperature	100.0	C
Pressure	101.3	kPa
Molar Flow	55.51	kgmole/h

coal		
Temperature	25.00	C
Pressure	8000	kPa
Molar Flow	90.27	kgmole/h

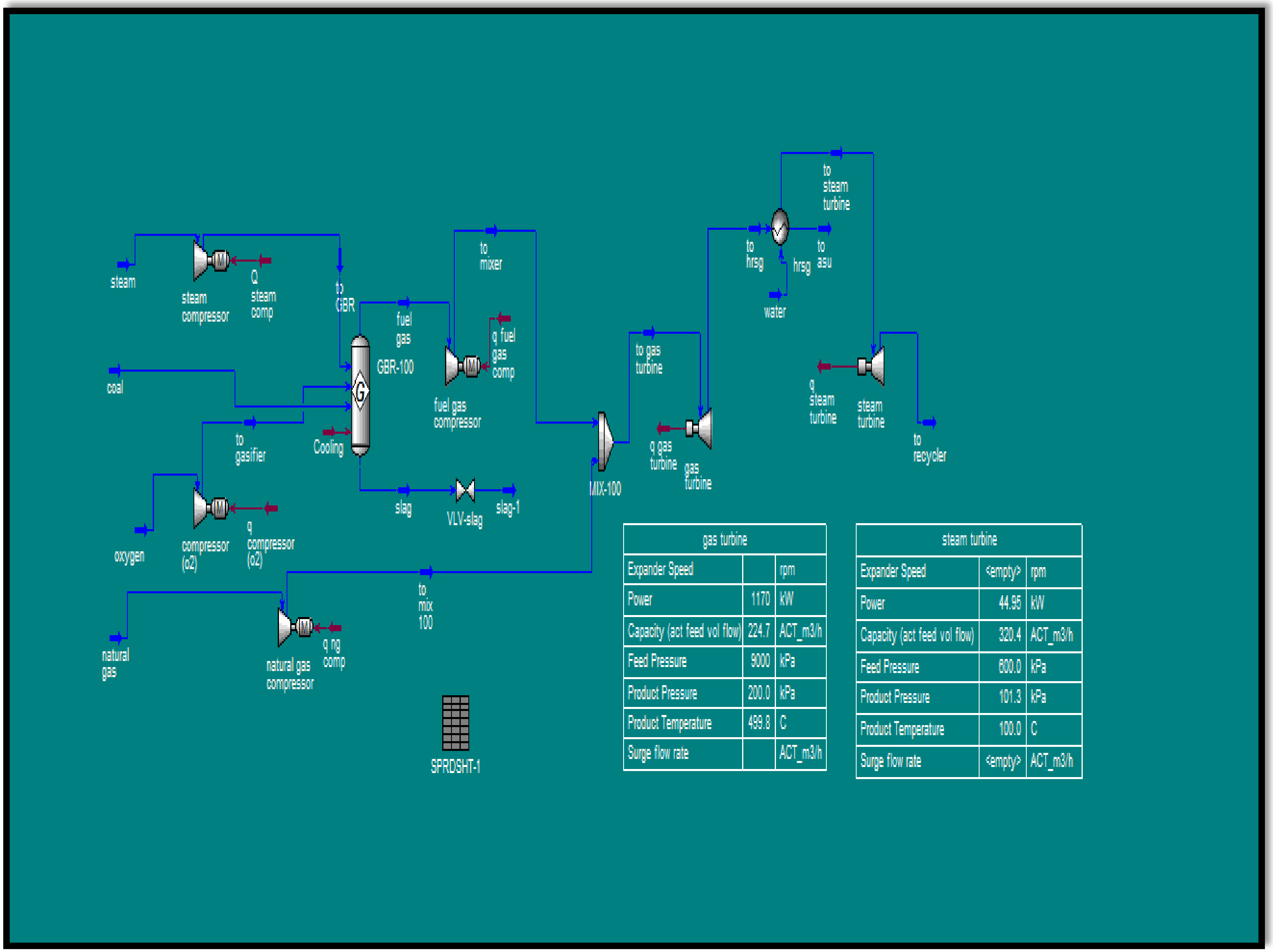
oxygen		
Temperature	25.00	C
Pressure	101.3	kPa
Molar Flow	31.25	kgmole/h

natural gas		
Temperature	25.00	C
Pressure	101.3	kPa
Molar Flow	62.33	kgmole/h

GBR-100		
Separator Type		
Vessel Temperature	1200	C
Vessel Pressure	8000	kPa
Vapour Molar Flow	137.5	kgmole/h
Liquid Molar Flow	0.0000	kgmole/h
Heat Flow	-9.142e+008	kJ/h

MIX-100		
Product Molar Flow	199.9	kgmole/h
Product Mass Flow	4000	kg/h
Product Volume Flow	7.544	m3/h
Product Temperature	928.7	C
Product Pressure	9000	kPa
Equalize Pressures	Yes	

Fig. 5.40: Optimized PFD with tabulated data for Coal-Natural Gas combination: Gasifier details



gas turbine		
Expander Speed		rpm
Power	1170	kW
Capacity (act feed vol flow)	224.7	ACT_m3/h
Feed Pressure	9000	kPa
Product Pressure	200.0	kPa
Product Temperature	499.8	C
Surge flow rate		ACT_m3/h

steam turbine		
Expander Speed	<empty>	rpm
Power	44.95	kW
Capacity (act feed vol flow)	320.4	ACT_m3/h
Feed Pressure	600.0	kPa
Product Pressure	101.3	kPa
Product Temperature	100.0	C
Surge flow rate	<empty>	ACT_m3/h

Fig. 5.41: Optimized PFD with tabulated data for Coal-Natural Gas combination: Turbine details

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CHAPTER -6

OPTIMIZATION OF GAS TURBINE OPERATED ON BIOMASS GASIFICATION

A simulation study using Aspen HYSYS® software tool has been carried out to arrive at the biomass derived power output of a gas turbine under various conditions as well as to perform changes in the fuel gas system for its augmentation. The results show that, the available fuel gas obtained from the biomass can be optimally used for the enhanced power generation in the gas turbine. The optimal process operating parameters also lead to improved gasifier efficiencies and heat recovery rendering a competitive alternative to conventional coal feed thermal power systems. A modular simulation user model of gasifier is also developed in Visual Basic. This model can be used for coal and biomass gasification process using downdraft gasifier model. The developed model can be embedded into commercial simulators. Hydrodynamic design of these gasifiers is also attempted using AutoCAD. Use of biomass generated syngas for feed to gas turbine, development of indigenous gasifier, and mechanical design of the developed gasifier model are innovative features of the present chapter.

Keywords: biomass; gasification; gas turbines; mathematical optimization; computer simulation; clean power production process, modular simulation, user model, mechanical design

6.1 INTRODUCTION

Energy production in industry is a resource-intensive and complex process. Decision support tools and mechanism need to be in place to allow consistent economic and operational growth. For this, one must consider the available resources in actual operations and market economy. Process simulation of a plant is a set of equations that describe the operations of the plant and predict its performances. This set of equations includes material and energy balances, rate equations, and equilibrium relations. The material balances describe the conservation of mass in the individual units of the process, and the energy balance equations describe the conservation of energy in these units. In the material balances, there are terms that describe the rate of conversion of components by chemical reactions. These terms are given by the rate equations from chemical kinetics. In energy balances, there are terms that describe the exchange in energy with the surroundings and the work done by the unit. The energy exchange is described by rate equations for heat transfer, and the work performed is described by the method used for fluid movement, e.g. compressor.

The aim of the present study is to evaluate the performance of biomass gasification reactor. We have analyzed the results of enhancement of gasifier efficiency on power generation by using the gasification fuel gas as the inlet to the gas turbine. A different approach is tried here to use the conditioned fuel gas directly as the gas turbine input rather than generating steam and using the same in steam turbine [1], which is generally adopted in many co-generation plants [2]. It is reported to have thermal efficiencies in the range of 25-30 % for furnaces and boilers using biomass feed stocks and efforts are being made to use IGCC [3, 4] and other techniques for improvisation in the efficiency using coal as the fuel [5]. As it is stated that, quality enhancement of synthesis gas will help use the same for many applications, including power production [6], many attempts are made to use this enhanced gas for production of chemicals [7, 8]. An attempt is made here to simulate the performance for power production, which is not reported earlier for larger production capacities [9]. Enhancement of gasifier efficiency as well as use of the gas generated from the renewable fuel for power production at large scale are the main objectives of the present work.

6.1.1 Resources of Biomass as Biofuel

Biomass encompasses any plant derived organic matter available on a renewable basis, including dedicated energy crops and trees, agricultural food and feed crops, agricultural crop wastes and residues, wood wastes and residues, aquatic plants, animal wastes, municipal wastes, and other waste materials. Handling technologies, collection logistics and infrastructure are important aspects of the biomass resource supply chain.

6.1.2 Benefits of Biomass

6.1.2.1 Reduced Air Pollution: Like other forms of renewable energy, such as wind or solar, biomass resources produce less emissions than their fossil fuel counterparts. Biomass contains less sulfur than coal, and consequently produces less SO_2. Emissions of NO_x are usually lower as well.

6.1.2.2 Reduced animal, food processing and municipal wastes: Anaerobic digestion can be used to convert wastes from livestock, food processing and households into energy. Using this biomass as energy can yield the following benefits: production of heat or electricity, odor reduction, reduced risk of water contamination, and reduced exposure to disease-causing organisms.

6.1.2.3 Reduction in landfills: A portion of landfills consists of woody biomass from construction, lumber mill activities, disposal of wooden pallets, etc. Wastes from food processing, paper industries and household garbage also contain organic matter that could be converted to energy. Using these materials to create energy means less landfill space is needed.

6.1.2.4 Lowering risk of wildfire: The risk of catastrophic wildfire can be reduced by removing small diameter trees that act as a fuel for the flames. Preventing wildfires can improve water quality. Wildfires reduce the ability of soil to absorb water that leads to increased debris and sediments in the riparian area.

6.1.2.5 Watershed quality enhancement: Reducing waste flows from livestock; food processing and city sanitation services can contribute to improved water quality [10].

6.1.3 Power Generation

The Combined Cycle is a generic type of plant that uses a gas turbine (GT) to produce electric or mechanical power and whose exhaust is used in a heat recovery steam generator (HRSG) that produces steam at different pressure levels [12]. The steam can be used in steam turbines for producing additional electricity or mechanical power and/or for the supply of heat loads in a process plant. The design of a power plant needs the optimal configuration of process operations and parameters, which can lead to the most economic design. These methods are briefly reviewed as follows:

6.1.4 Thermodynamic Approach

The traditional way of designing power plants is to maximize the thermal efficiency of the plant. For this purpose analysis methods based on both the first and the second law of thermodynamics have been extensively discussed in literature [13]. The analysis reveals the thermal inefficiencies of the various subsystems of the plant. Once the inefficiencies have been identified, heuristic rules are applied to improve the performance of the plant. These heuristics form the basis for both parameter and structural modifications to the plant. The capital cost of the plant is assessed after the thermally best design is achieved.

6.1.5 Thermoeconomic Approach

This is an extension of the thermodynamic approach. The capital cost of the units and the prices of product streams of the units are included in the second law analysis model of the plant. This approach tries to address the trade-off between thermal efficiency and capital expenditure. The model is subjected to NLP-optimization for finding the most economic operating parameters [14]. Although this approach provides the economically best parameters, the methodology still relies on trial-and-error, when addressing structural changes to the existing process.

6.1.6 Thermochemical Combustion Process: Gasification

Gasification requires biomass to undergo partial oxidation at high temperature to produce a gas containing carbon monoxide, hydrogen, methane as well as carbon dioxide, nitrogen (from the air, if used) and water vapour. Air or oxygen may be used for the oxidation and steam may be added. Gasification reactions are mostly endothermic (requiring heat), whereas the combustion reactions are exothermic (releasing heat). Heat is not the product in the gasification process, and in fact must be added or produced by combustion of some of the fuel, but the result is that the biomass is transformed into a gaseous fuel. Gas is easier to handle than solid fuel and burns at higher temperatures. The gasification chamber can be the same as that used for combustion. Whether gasification or combustion occurs depends on the oxygen/fuel ratio: Therefore, approximately 1/3 of the oxygen is required for a gasification process. Gasification converts solid organic material into a combustible gas that is generally used in an engine or gas turbine.

6.1.7 Hydrogen from Biomass

Thermal, steam and partial oxidation gasification technologies are under development around the world [16, 17, 18]. Feedstock include agricultural and forest product residues of hard wood, soft wood and herbaceous species. Thermal gasification is essentially high-rate pyrolysis carried out in the temperature range of 600–1000°C in the gasifiers.

The reaction is as follows:

$$\text{Biomass} + O_2 \rightarrow CO + H_2 + CO_2 + \text{Heat}$$

Other relevant gasifier types are bubbling fluid beds and the high-pressure high-temperature slurry-fed entrained flow gasifier.

However, all these gasifiers have included significant gas conditioning along with the removal of tars and inorganic impurities and the subsequent conversion of CO to H_2 by water gas shift reaction.

$$CO + H_2 \rightarrow CO_2 + H_2O$$

A study of agriculture residue steam gasification in a gasifier reveals that at 805°C, smaller particle size yields more hydrogen than that of at higher temperatures [19]. Catalytic steam gasification of biomass has also been studied in a bench-scale plant gasifier and a secondary fixed-bed catalytic reactor. The catalytic converter using different steam-reforming nickel catalysts and dolomite has been tested over a temperature range of 660–830°C. Fresh catalyst at the highest temperature yields 60% by volume of hydrogen [20].

6.2. MODELING AND SIMULATION OF GASIFICATION

The model described in the figure 6.1 indicates the biomass gasification process used here where the biomass decomposes to volatiles, gases and char. The volatiles and gases further react with char to produce different types of volatiles, gases and char where the compositions are different. The primary products participate in secondary interactions which result in a modified final product distribution.

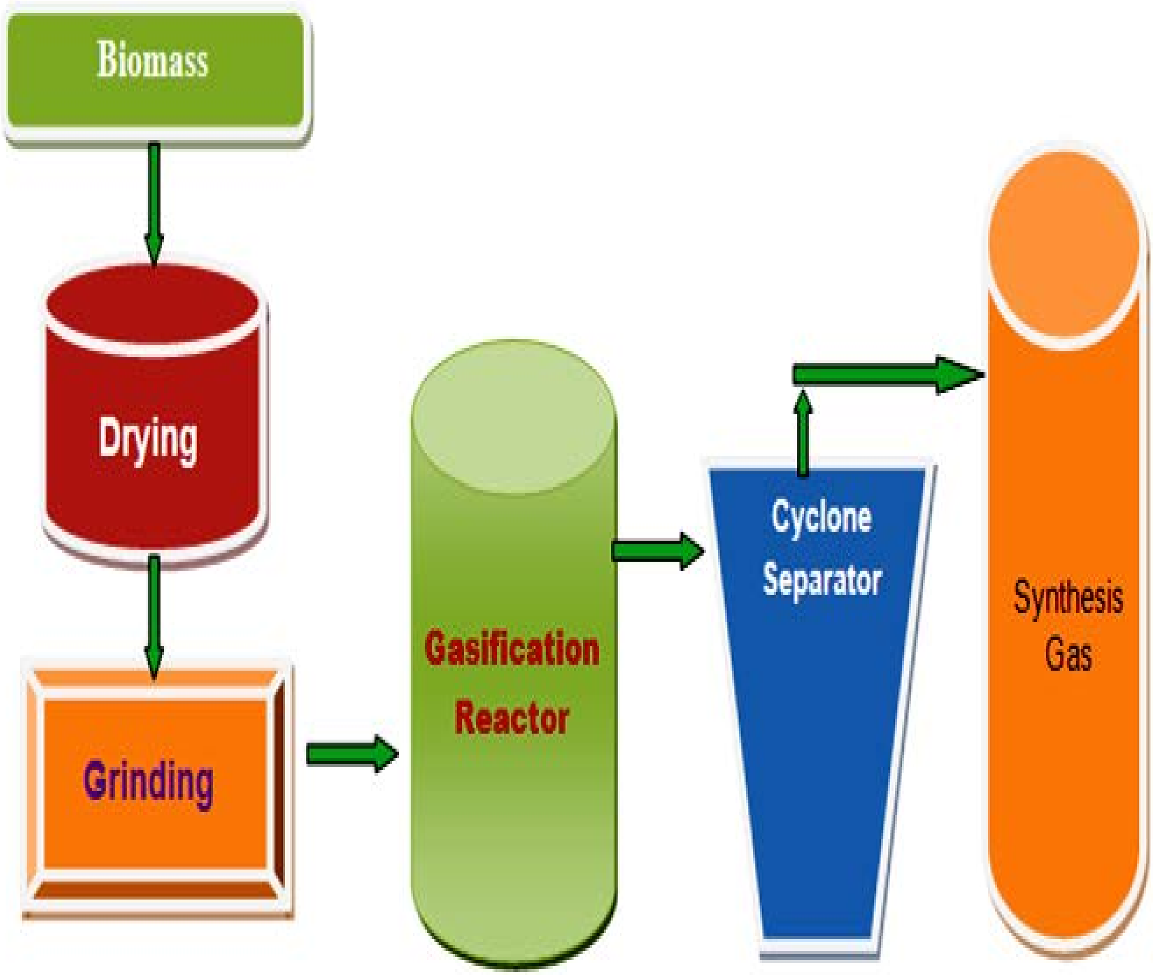


Fig 6.1: Fuel gas generation using biomass

We modeled the biomass gasification process kinetically and the governing equations based on the mechanism shown in the figure above are as follows:

$$\frac{dC_b^{n1}}{dt} = -K_1 C_b^{n1} - K_2 C_b^{n1} \text{..................} \quad (1)$$

$$\frac{dC_g}{dt} = K_1 C_b^{n1} - K_3 C_{G1}^{n2}\, C_{C1}^{n3} \;\ldots\ldots\ldots\ldots\ldots\ldots \text{(2)}$$

$$\frac{dC_c}{dt} = K_2 C_b^{n1} - K_3 C_{G1}^{n2}\, C_{C1}^{n3} \ldots\ldots\ldots\ldots\ldots\ldots \text{(3)}$$

Where

$$\mathrm{K_1} = \mathrm{A_1}\ \exp\left(\frac{-\mathrm{E_1}}{\mathrm{RT}}\right) \qquad \mathrm{K_2} = \mathrm{A_2}\ \exp\left(\frac{-\mathrm{E_2}}{\mathrm{RT}}\right) \qquad \mathrm{K_3} = \mathrm{A_3}\ \exp\left(\frac{-\mathrm{E_3}}{\mathrm{RT}}\right)$$

A carefully planned controlled set of experiments were carried out on a bench scale unit to generate rate information for the specific biomass used in this simulation study and the values are as follows:

$A_{1=}$ 1.489 x 10^{-3} S^{-1}, $A_{2=}$ 4.755 x 10^{-3} S^{-1}, $A_{3=}$ 11.521 x 10^{5} S^{-1}

E_1= 21 kJ/mol, E_2= 49 kJ/mol, and E_3= 119 kJ/mol.

The biomass used here is agriculture waste of sugar cane crop. The ultimate analysis (wt%) of the biomass used is as given in table 6.1.

Table 6.1: Biomass ultimate analysis (wt %)

C	H	O	N	S	A
49.09	**5.5**	**37.23**	**0.97**	**0.13**	**7.1**

Equations 1 through 3 are used at isothermal conditions with different temperatures from 599^{o}C to 1499^{o}C with 10^{o}C as step size for the optimal solutions. The above rate information is used to determine the product outlets from the biomass gasifier which then enter into conditioning skid where char is removed. This clear gas is now used in the gas turbine for the power generation.

6.3 MODEL OF POWER PLANT

The model used here consists of choosing proper gas stream, selection of components of Gas Turbine with design parameters and then simulation of the power plant. The details of each step are described below.

6.3.1. Gas Stream

The model for the gas turbine requires feed stream which contain:

- Gaseous fuel (containing CO, H_{2}, CH_{4}, etc.).
- O_2 in pure form or air
- Exhaust gas components, including products of combustion and dissociation reactions

The model of a biomass based power plant with allied processes is well illustrated in figure 2. The stream definition contains *N*=6 variables (where *N* is the number of components for a given gas stream). The parameters which we need are *F*, *H*, *T*, *P*, *h*, *s*, y_i (i=1,…,*N*) and respectively represent molar flow, enthalpy flow, temperature, pressure, specific enthalpy, specific entropy, and mole fractions.

A typical composition of raw gas at the outlet from gasifier is provided in table 6.2.

Table 6.2: Gasifier outlet gas analysis (mol %)

CO	**H_2**	**CO_2**	**N_2**	**CH_4**	**Others**
26.35	**51.69**	**21.96**	**1.8**	**1**	**0.2**

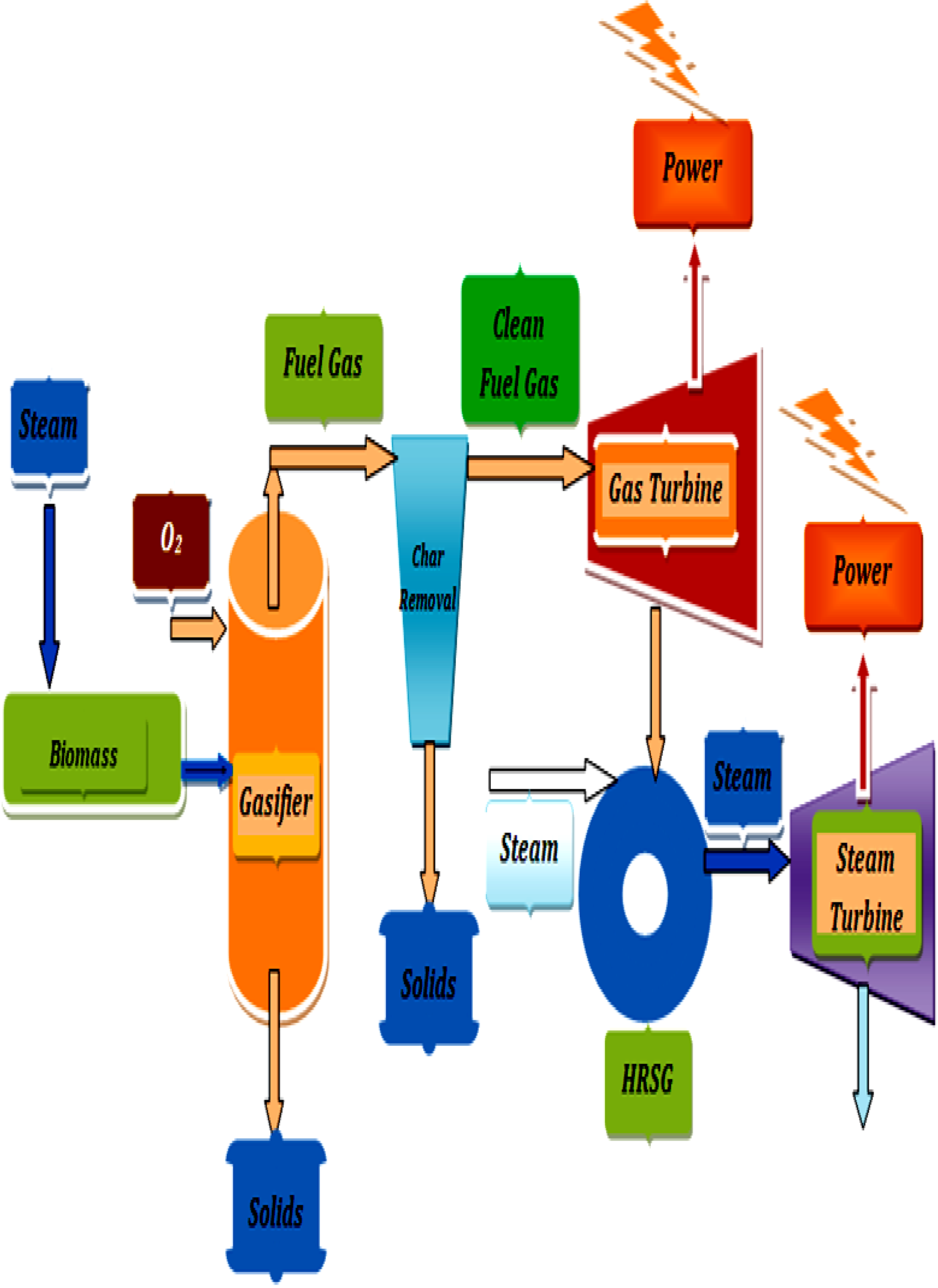


Fig.6.2: Overview of a gasifier for power production with relevant processes

6.3.2. Gas Turbine

The model of gas turbine consists of the following three sections:

- a compressor;
- a combustion chamber with a pre-mixer for air/oxygen and fuel; and
- an expansion section.

We have simulated a full model for a gas turbine including these subsections and obtained the relationship between work produced by the expansion section, work required by the compressor section and the external load. In modeling the combustion chamber, first we have considered the mixing of air from the compressor section with fuel and then a combustion reaction section. The combustor model requires energy balance and reaction equilibrium equations to get the temperature and composition of the combustion products. The operating parameters for the four gas turbines are shown in table 6.3.

Table 6.3: Gas Turbine operating parameters

Design Capacity (m^3/hr)	**Pressure (barg)**		**Temperature (^OC)**	
	Operating	**Design**	**Operating**	**Design**
11.37	7.5	13.5	50	95

The simulation is also carried out at various humidity conditions for finding the model robustness and proving the validity for reproducing the results in different conditions. The winter conditions used for the model validation are provided in the table 6.4.

Table 6.4: Effect of humidity on power generation-winter conditions

Gas Analysis, % Humidity	**Power Generation in GTG 1-4, kW**
17	124993.5
35	125003.0
50	124993.5

Table 6.5: Parameters for modeling of Gas Turbine and enhanced power generation calculations

Turbine Parameters	Units	GTG1	GTG2	GTG3	GTG4
Fuel Gas mass Flowrate	kg/hr	8494	8494	8494	5518
Vapour Fraction	-	1	1	1	1
Liquid Fraction	-	0	0	0	0
Temperature	^{0}C	20.04	20.04	20.04	20.04
Pressure	KPa	2301	2301	2301	2301
LHV	KJ/kg	47310	47310	47310	47310
HC Dew Point (Gas)	^{0}C	-39.63	-39.63	-39.63	-39.63
Water Dew Point (Gas)	^{0}C	-260.5	-260.5	-260.5	-260.5
Compressor Power (consumed)	kJ/hr	283400000	283400000	283400000	184000000

Heater Power (consumed)	kJ/hr	0	0	1090800	0
Turbine Power (Generate)	kJ/hr	412000000	412000000	412000000	274900000
Total Power Generation	kJ/hr	128600000	128600000	127509200	90900000
	kW	35722	35722	35419	25250
	MW	**132.114**			

The complete set of parameters used in modeling of the gas turbine is illustrated in table 6.5. Table 6.5 also indicates the achievement of present study for enhancement of power production capacity.

6.4 SIMULATION OF A FULL GAS TURBINE (GT)

The equipment sections and streams needed to model an open-cycle gas turbine are similar to those used in the earlier study on coal [21, 22]. The inlet/outlet conditions and operating parameters are however different for the biomass feed used here and yields different optimal parameters. More specifically, the model includes:

1. The compressor section where air is compressed and then mixed with fuel

2. The combustion chamber where fuel is burned with an excess of oxygen at high temperature of 1421°C and high pressure of 3.9 MPa; and

3. The expansion section where the combustion gases are expanded to produce shaft work for electric power generation or mechanical power, and to drive the compressor section of the gas turbine. The essential data used for the gas turbine simulation are provided in the table 6.6.

Table 6.6: Data for simulation of the power plant

Process	Parameters	Values
Turbine of GT	**Power**	**100MW**
	Inlet Temperature	**1421 °C**
	Isentropic Efficiency	**93.3 %**
GT Compressor	**Pressure Ratio**	**9.09**
	Isentropic Efficiency	**59.99 %**

As the combustion chamber model is complex, we first simulated this equipment in its standalone fashion. This was the most difficult subsection to converge since the equations relating the combustion temperature and composition and dissociation reactions are highly non-linear [23]. The chemical reactions involved in the process are very complex as many components are involved, and there is a network of irreversible consecutive and competitive reactions. The model uses a relatively simple approach to represent the reaction set and some trace reaction products, like CS_2 are not considered. The reactors are modeled with the Aspen HYSYS®. The complete simulated plant is shown in figure 6.3.

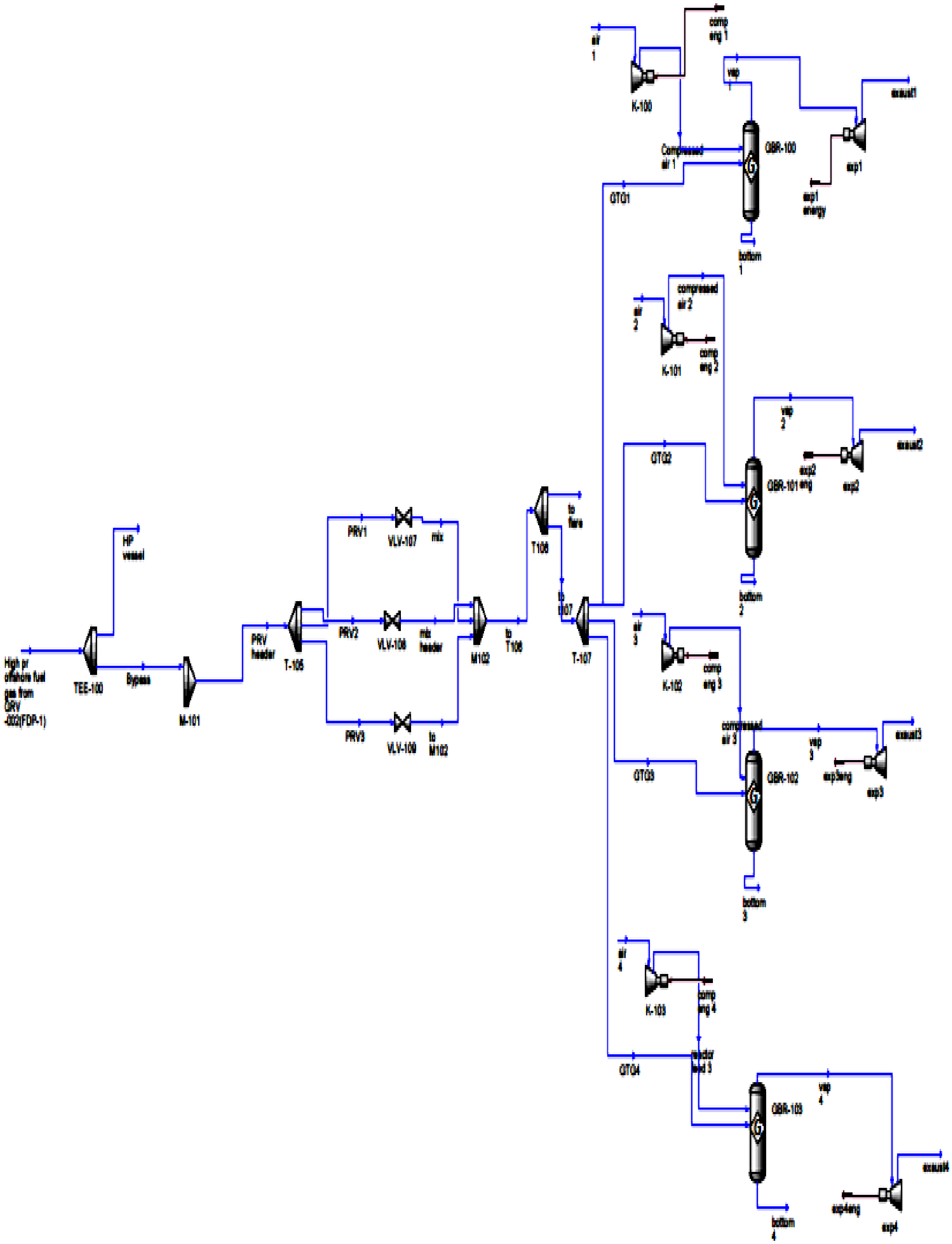


Fig. 6.3 Simulation of biomass generated fuel gas operated gas turbines

6.5 RESULTS AND DISCUSSION

As a result of the simulation studies and adjustment of operating parameters, the power generation in each set of four GTGs is enhanced to 125 MW from 100 MW. The parameters for power production enhancement are provided in table 6.7.

Table 6.7: Enhancement in power generation in existing gas turbines

Power Generation	Gas Flow NM^3/hr	Temperature, ^oC	Pressure, MPa	Heat Savings, kW	Thermal Efficiency, %
100 MW	**41590**	**1529**	**3.9**	**0.0**	**45.32**
125 MW	**55630**	**1421**	**3.9**	**900**	**59.99**

The simulation study shows that maximum possible power is generated with 55630 NM^3/hr of fuel gas flow bypassing the heater skid which saves energy on heating the gas to the extent of 900 kWh electric power and maximum possible power generation in four GTGs is further enhanced from 125 MW to approx 132 MW. This in total adds a power generation of 28-30 MW for a set of four GTGs, which is a significant achievement of this study. The details of higher power achievement along with parameters used for Gas Turbine model are presented in table 6.5. The results are shown in table 6.8 and are illustrated in fig. 6.4.

Table 6.8: Effect of fuel gas flow rate on power generation, t=1421°C, P=3.9 MPa

Gas Flow NM^3/hr	**45500**	**50500**	**55630**	**57500**	**60500**
Power output, MW	**113.72**	**122.5**	**131.9**	**129.45**	**130.21**
Heater savings, kW	**490**	**530**	**900**	**1089**	**1145**

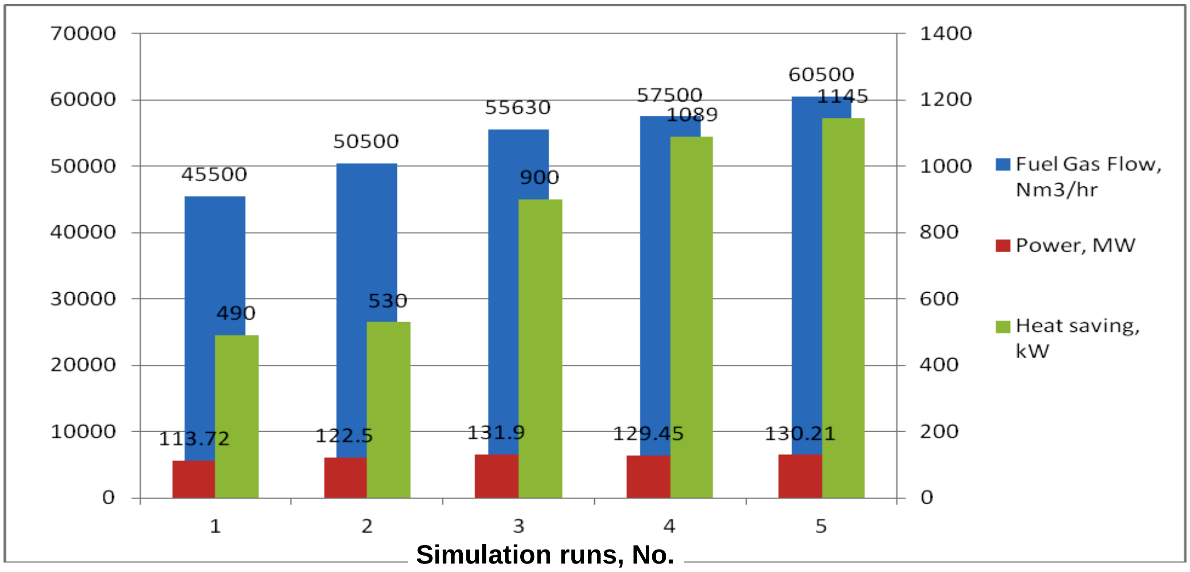


Fig.6.4: Effect of fuel gas flow variation on power output, and heat savings by avoiding raw gas heater skid

Increasing gas flow beyond 55630 Nm^3/hr saves more energy on preheating in heater skid, but decreases the power output at operating temperature and pressure. The effect of parameters on power generation has been reported earlier [24, 25]. For this model, the probable causes for the same may be the radiation heat losses, loss of thermal energy along with exhaust gases, altered kinetics and hence composition of gas and heavy pressure drops. The simulation also shows that we could enhance the gasifier efficiency to 59% from 45 % [26] by maintaining inlet temperature below 1500°C. The fuel gas analysis and the gasifier efficiency comparisons are shown in figs. 6.5 and 6.6.

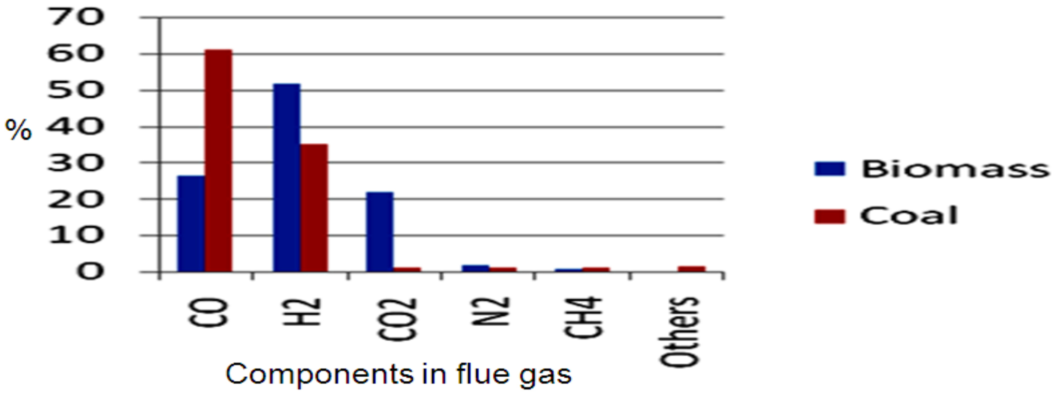


Fig. 6.5: Comparison of biomass and coal gasification fuel gas analysis

Fig. 6.6 shows the simulation runs for various gas heat values indicating that higher gasifier efficiencies can be realised for high heat values. For the feed considered here, the line number 4 represents the achievable efficiency whereas line 6 indicates earlier result on coal [26]. The simulation also shows an opportunity to enhance the efficiency further when higher gas heat values can be realised. This may be possible by choosing appropriate biomass or blending with other fuels. Higher efficiencies help to complete conversion of CO and NOx, which in turn reduces pollution and makes this a process of clean power production. Modelling the reaction kinetics accurately provides fuel gas with higher heat values. Results in table 6.8 indicate the achieved composition of fuel gas. The recent studies are also reporting the same approach [27].

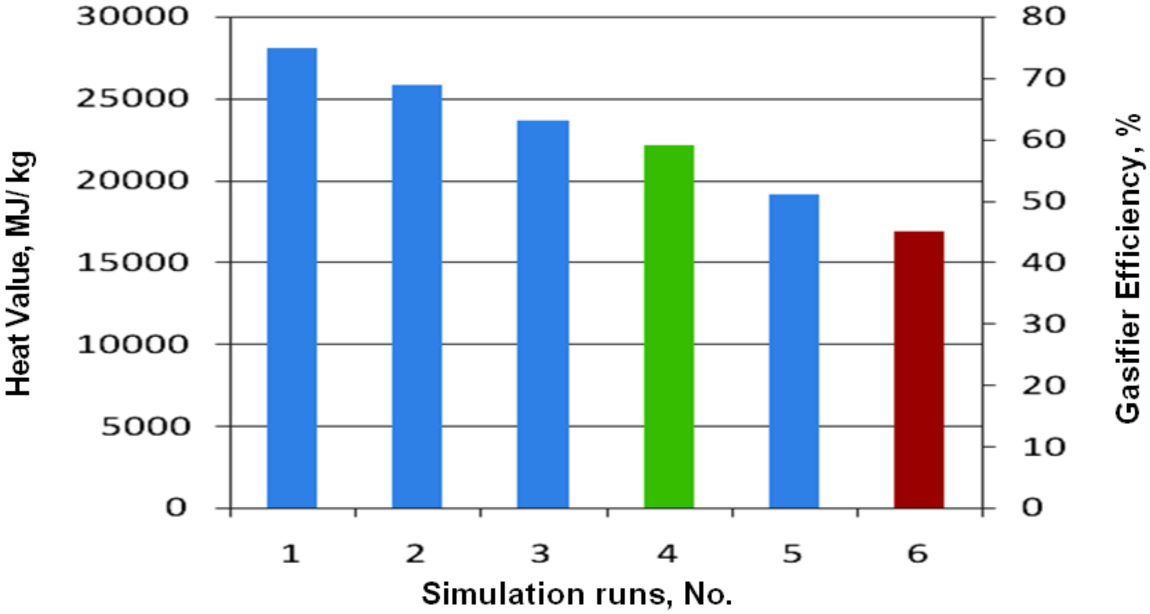


Fig. 6.6: Comparison of biomass gasifier efficiency, simulation run 4 indicating achievement of the present study compared to earlier reported indicated by sixth column

As no data for the considered biomass at large scale is available, a comparison is made with fuel gas of coal gasification output in table 6.9. The results prove that the present work provides opportunities to use the biomass generated fuel gas for power generation as a safe substitute to coal gasification process. The reliability of power generation has also been tested and is presented in figure 6.7.

Table 6.9: Fuel gas composition, (mol %)

Fuel Type	Fuel gas composition, (mol %)					
	CO	H_2	CO_2	N_2	CH_4	Others
Biomass	26.35	51.69	21.96	1.8	1	0.2
Coal	61	35	1	1	1	1.5

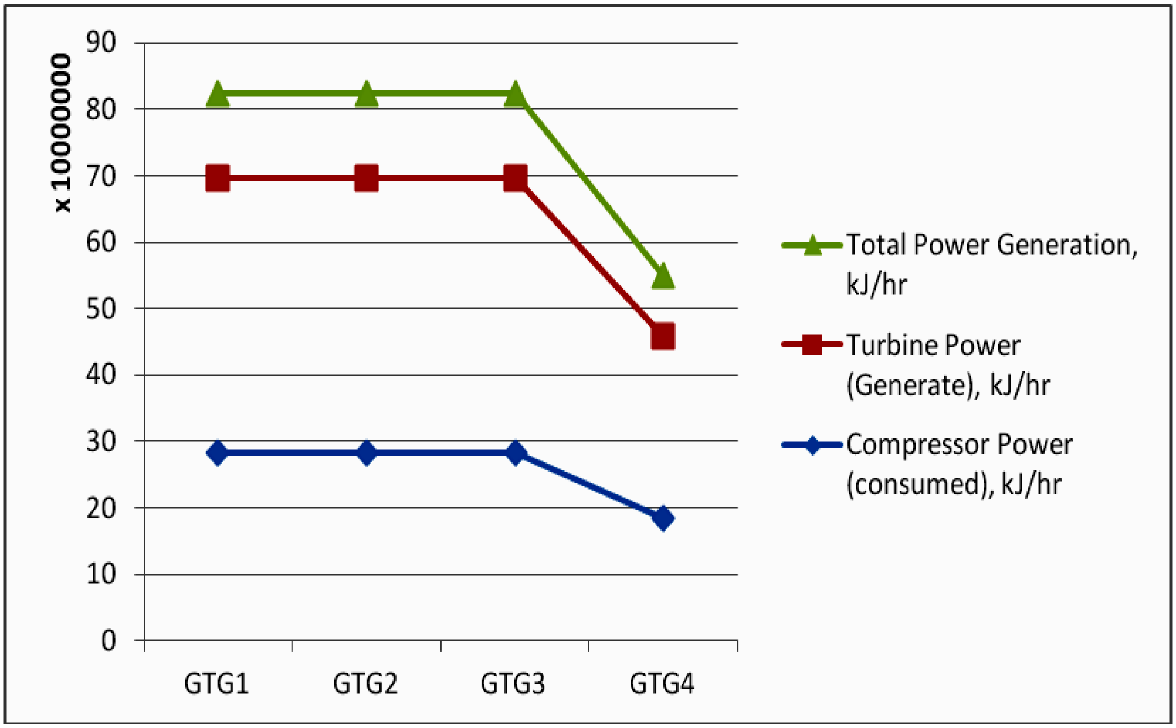


Fig 6.7: Comparison of biomass gasifier power generation in four gas turbines: a reliability study for continuous power generation

6.6 DEVELOPMENT OF USER MODEL FOR MODULAR SIMULATION OF BIOMASS GASIFICATION PROCESS

As the standard commercial simulators do not have specified gasifiers for biomass gasification system, we need to model them with various reactor types available in the existing simulators. This has been tried in the present study in chapters 1 through 5 as well as early part of chapter 6. While suggesting and implementing innovative ideas and approaches throughout the present study, it was decided to develop an indigenous modular simulation which will have our design specification criteria along with our own voluminous data as back end. Having a very brief of required information from literature for design, we will start developing the user model.

6.6.1 Theory of Gasification

The production of generator gas (producer gas) called gasification, is partial combustion of solid fuel (biomass) and takes place at temperature of about 1000ºC. The reactor is called a gasifier. The combustion products from complete combustion of biomass generally contain nitrogen, water vapor, carbon dioxide and surplus of oxygen. However in gasification where there is a surplus of solid fuel (incomplete combustion) the product of combustion are combustible gases like Carbon monoxide (CO), Hydrogen (H_2) and traces of Methane and non-useful products like tar and dust. [10]. Details of gasification is already elaborated in other parts of this thesis.

6.6.2 Types of Gasifiers [10]

A variety of biomass gasifier types have been developed. They can be grouped into four major classifications: fixed-bed updraft, fixed-bed downdraft, bubbling fluidized-bed and circulating fluidized bed. Differentiation is based on the means of supporting the biomass in the reactor vessel, the direction of flow of both the biomass and oxidant, and the way heat is supplied to the reactor. This analysis of gasifiers will help in proper selection of development of model for our present study.

Table 6.10: Gasifier classifications

Gasifier Type	**Flow Direction**		**Support**	**Heat Source**
	Fuel	Oxidant		
Updraft Fixed Bed	Down	Up	Grate	Combustion of char
Downdraft Fixed Bed	Down	Down	Grate	Partial combustion of volatiles
Bubbling Fluidized Bed	Up	Up	None	Partial combustion of volatiles and char
Circulating Fluidized Bed	Up	Up	None	Partial combustion of volatiles and char

Table 6.11: Advantages and disadvantages of different types of gasifiers

Sl. No.	**Gasifier Type**	**Advantages**	**Disadvantages**
1	Updraft	a) small pressure drop b) good thermal efficiency c) little tendency towards slag formation	a) great sensitivity to tar and moisture content of fuel b) relatively long time required for start-up of IC engine c) poor reaction capability with heavy gas load
2	Downdraft	a) flexible adaptation of gas production to load b) low sensitivity to charcoal dust and tar content of fuel	a) Design tends to be tall b) Not feasible for very small particle size of fuel.
3	Cross draft	a) short design height b) very fast response time to load c) flexible gas production	a) very high sensitivity to slag formation b) high pressure drop

6.6.3 Gasification Zones

Following zones are considered for development of model. These zones are explained in brief below [10].

6.6.3.1 Pyrolysis

Pyrolysis is the application of heat to raw biomass, in an absence of air, so as to break it down into charcoal and various tar gasses and liquids.

6.6.3.2 Reduction

Reduction is the process stripping of oxygen atoms off completely combusted hydrocarbon (HC) molecules, so as to return the molecules to forms that can burn again. Reduction is the direct reverse process of combustion.

6.6.3.3 Combustion and Drying

Combustion is what generates the heat to run reduction, as well as the CO_2 and H_2O to be reduced in Reduction. Combustion can be fuelled by either the tar gasses or char from Pyrolysis.

6.6.4 DESIGN AND MODELLING

6.6.4.1 Design of a Down Draft Gasifier

Downdraft gasifiers are one among the fixed bed gasification system. Downdraft gasification technology has an increased interest among research worldwide due to the possibility to produce mechanical and electrical power from biomass in small scale to an affordable price [16].

6.6.4.2 Design Parameters

There are several factors to consider in designing a Gasifier. Proper consideration of these different factors will be of great help in order with the desired design of the reactor and its desired performance. As given below, the different factors that need to be considered in designing a gasifier using different biomass as fuel are:

6.6.4.3 Types of Reactors

The operating performance of the reactor basically depends on the type of the reactor used [16, 27].

6.6.4.4 Cross Sectional Area of the Reactor

This is the area in which biomass is burned and this is where the fuel is gasified.

6.6.4.5 Height of the Reactor

The height of the reactor determines the time the gasifier can be operated continuously and the amount of gas that can be produced for a fixed column reactor.

6.6.4.6 Thickness of the Bed

The thickness of the fuel bed is only considered when designing a cross-draft gasifier. It is the same as that of the height of the reactor in the down-draft gasifier.

6.6.4.7 Fan Airflow and Pressure

The fan provides the necessary airflow that is needed for the gasification of biomass fuels. They are available in AC or DC.

6.6.4.8 Insulation for the Reactor

The gasifier reactor needs to be properly insulated for two reasons: First, this will provide better conversion of fuel into gas.

6.6.4.9 Location of Firing the Fuel

Fuel can be fired in the reactor in different ways. For fixed bed gasifiers, like the down-draft reactor, fuel can be fired starting from the top (Top Lit) or from the bottom (Bottom Lit) of the reactor.

6.6.4.10 Size and Location of the Char

The size of the chamber for carbonized biomass determines the frequency of unloading the char or the ash.

6.6.5 DESIGN CALCULATIONS FOR A DOWNDRAFT GASIFIER

Some important parameters considered in determining the appropriate size of the gasifier, taking into consideration the power output desired are presented here. The size of the reactor can be easily estimated by computing these parameters.

6.6.5.1 Energy Demand

This refers to the amount of heat that needs to be supplied by the reactor. This can be determined based on the amount of fuel to be gasified and/or water to be boiled and their corresponding specific energy needed.

The amount of energy needed to cook food can be calculated using the formula:

$$Q_n = \frac{M_f \text{ x } E_s}{T}$$

where:

Q_n - Energy needed, kcal/hr

M_f - Mass of Fuel, kg

E_s - Specific energy, kcal/kg

T - Gasifying time, hr

6.6.5.2 Fuel Demand: Energy Input

This refers to the amount of energy needed in terms of fuel to be fed into the reactor. This can be computed using the formula.

$$FCR = \frac{Q_n}{HV_f \times \xi_g}$$

where:

FCR - Fuel Consumption Rate, kg/hr

Q_n - Heat energy needed, Kcal/hr

HV_f - Heating Value of fuel, Kcal/kg

ξ_g - Gasifier efficiency, %

6.6.5.3 Reactor Diameter

This refers to the size of the reactor in terms of the diameter of the cross-section of the cylinder where fuel is being burned. This is a function of the amount of the fuel consumed per unit time (FCR) to the specific gasification rate (SGR). The reactor diameter can be computed using the formula,

$$D = \left(\frac{1.27x\ FCR}{SGR}\right)^{0,5}$$

where:

D - Diameter of reactor, m

FCR - Fuel Consumption Rate, kg/hr

SGR - Specific Gasification Rate of Biomass, (90 - 210 kg/m^2-hr)

6.6.5.4 Height of the Reactor

This refers to the total distance from the top and the bottom end of the reactor. This determines how long would the stove be operated in on loading of fuel. Basically, it is a function of a number of variables such as the required time to operate the gasifier (T), the specific gasification rate (SGR), and the density of the feed (ρ).

As shown below, the height of the reactor can be computed using the formula,

$$H = \frac{SGRxT}{\rho}$$

where:

H - Height of the reactor, m

SGR - Specific Gasification Rate of biomass, kg/m^2-hr

T - Time required to consume biomass, hr

ρ - Fuel density, kg/m^3

6.6.5.5 Amount of Air Needed for Gasification

This refers to the rate of flow of air needed to gasify biomass. This is very important in determining the size of the fan or of the blower needed for the reactor in gasifying rice husks. As shown, this can be simply determined using the rate of consumption of fuel, Fuel Consumption Rate (FCR), the stoichiometric air of fuel (SA), and the recommended equivalence ratio as 0.3 or 0.4. As shown, this can be computed using the formula,

$$AFR=\frac{\varepsilon\times FCR\times SA}{\rho_a}$$

where:

AFR - Air Flow Rate, m^3/hr

ε - Equivalence ratio, 0.25 to 0.4

FCR – Fuel Consumption Rate of Biomass, kg/hr

SA - Stoichiometric air of fuel

ρ_a - Air density, 1.25 kg/m^3

6.6.5.6 Superficial Air Velocity

This refers to the speed of air flow in the fuel bed. The velocity of air in the bed rice husks will cause channel formation, which may greatly affect gasification. The diameter of the reactor (D) and the airflow rate (AFR) determine the superficial velocity of air in the gasifier.

As shown, this can be computed using the formula,

$$VS = \frac{4xAFR}{D^2}$$

Where:

V_S - Superficial gas Velocity, m/s.

AFR - Air Flow Rate, m^3/hr.

D - Diameter of reactor, m.

6.6.5.7 Throat Diameter

This refers to the diameter of the throat inside the gasifier. This parameter can be calculated when the diameter of the reactor is known. Normally the throat diameter will be 1/3rd of the reactor diameter.

$$\boxed{D_t = (1/3) \times \text{Diameter of the reactor}}$$

Where, D_t = Diameter of throat

6.6.6 DESIGN OF GASIFIER IN VISUAL BASIC®

6.6.6.1 Introduction

Visual Basic® is an open-platform user program from Microsoft® Visual Studio. This is a front end Graphical User Interface (GUI) development programme providing many back end (data storage) operations, which eliminate many difficulties in manual design considerations. Use of combo box, textbox, label, etc is done in order to present the output parameters required to simulate the gasifier. Visual Basic is chosen as the programming language because the model developed in the language can be directly embedded in commercial chemical process simulation software such as Aspen Plus® and HYSYS®. FORTRAN® and Visual Basic are the two major input languages for the modular simulators. As all these software are based on Visual Basic platform, it was decided to use the same coding language for our study. The author is a well versed programmer in usage of Visual Basic and other back end programmes as MS-SQL® or Oracle®.

6.6.6.2 Steps in Development of User Model

First, the user is asked to choose a fuel, based on the selection of fuel from the list, various constants are generated. Then the user is asked to specify some important parameters needed for design calculations such as the time for gasification, mass flow rate desired etc. The constants such as calorific value, density of fuel at standard condition etc. are provided by using the developed modular simulation. After running the simulation, the results are displayed on the adjacent column. If the user is not satisfied with output, he/she can change the input and find an appropriate and desired output.

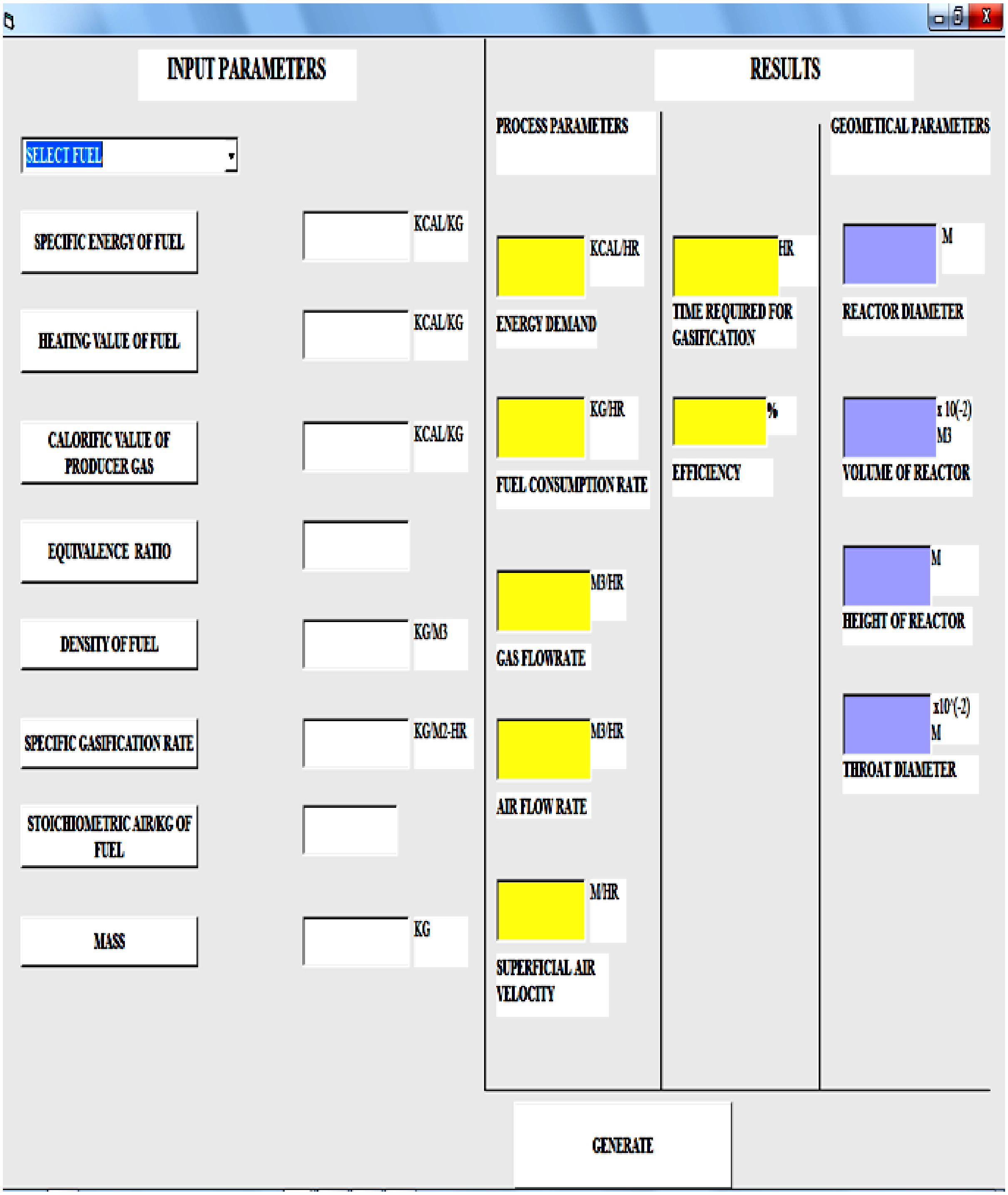


Fig 6.8: Visual Basic User Model for gasification process

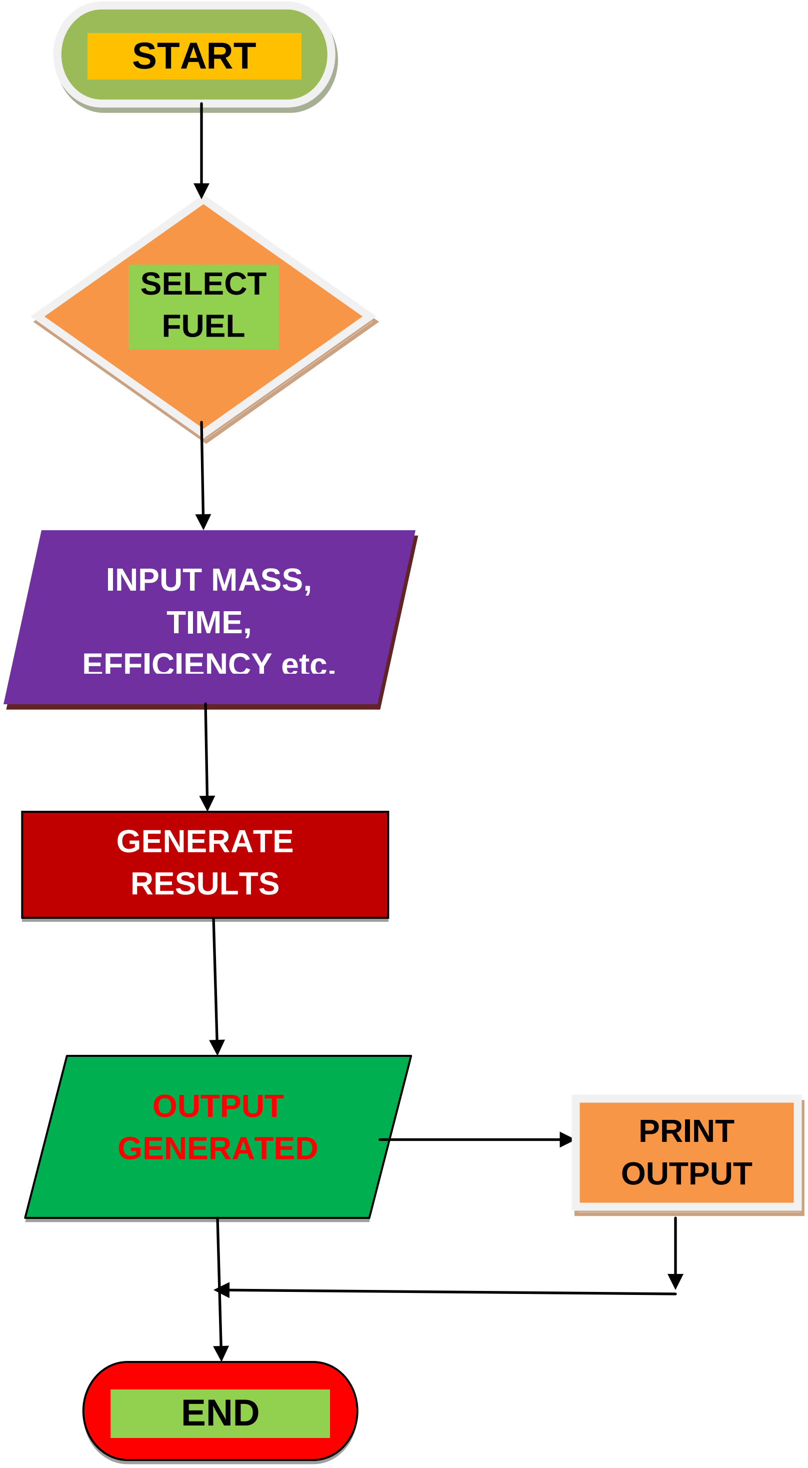


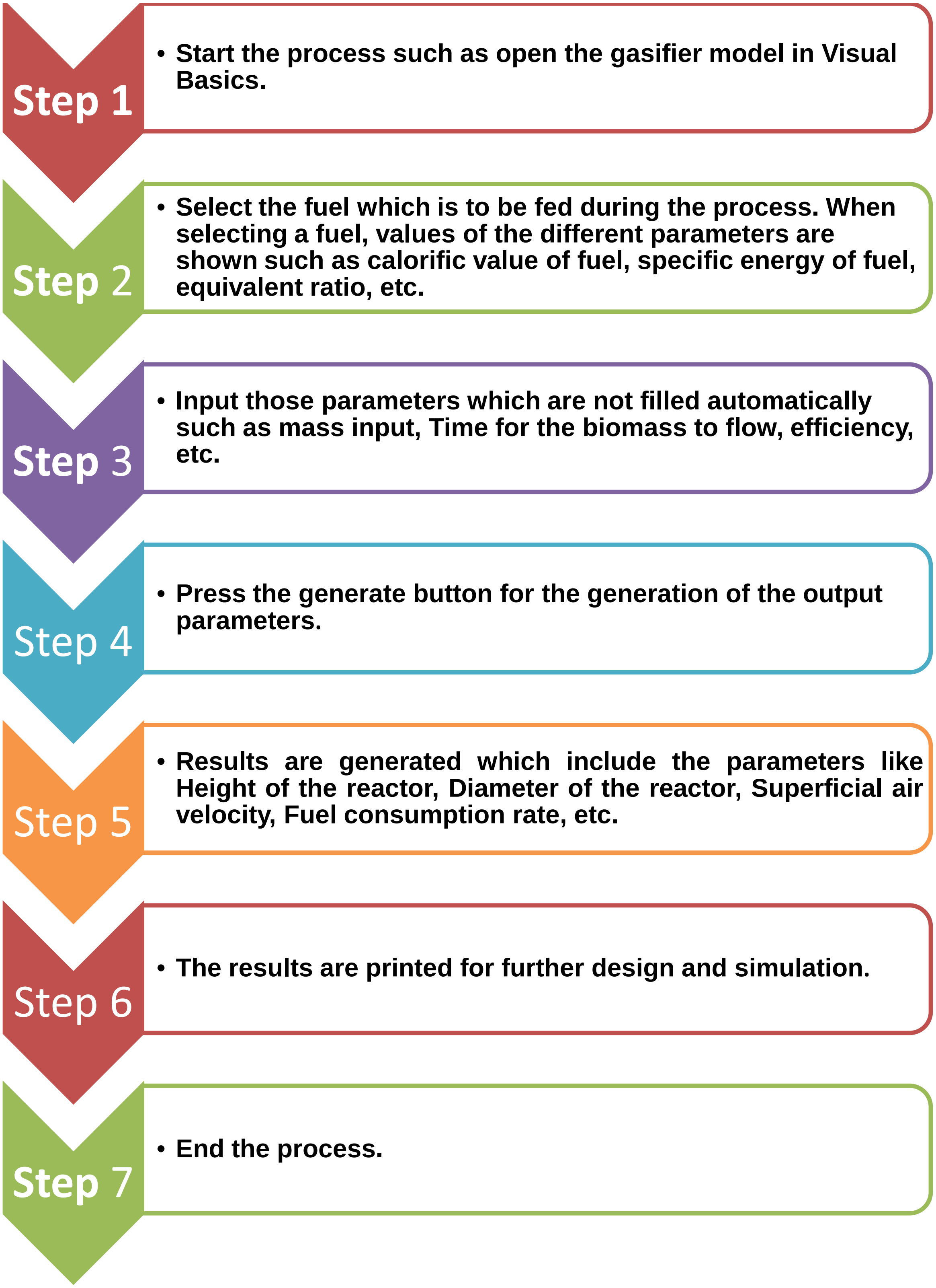
Fig 6.9: Process Flow Diagram for the user model development process

6.6.6.3 ALGORITHAM OF THE PROGRAM

The following algorithm is developed for the gasifier modular simulation model in Visual Basic:

- Start the process such as open the gasifier model in Visual Basic.
- Select the fuel which is to be fed during the process. When selecting a fuel, values of the different parameters are shown such as calorific value of fuel, specific energy of fuel, equivalent ratio, etc.
- Input those parameters which are not filled automatically such as mass input, Time for the biomass to flow, efficiency, etc.
- Press the generate button for the generation of the output parameters.
- Results are generated which include the parameters like Height of the reactor, Diameter of the reactor, Superficial air velocity, Fuel consumption rate, etc.
- The results are printed for further design and simulation.
- End the process.

Fig 6.10 shows the detailed steps to be followed by a user to develop a gasification modular simulation model.



Step 1

- Start the process such as open the gasifier model in Visual Basics.

Step 2

- Select the fuel which is to be fed during the process. When selecting a fuel, values of the different parameters are shown such as calorific value of fuel, specific energy of fuel, equivalent ratio, etc.

Step 3

- Input those parameters which are not filled automatically such as mass input, Time for the biomass to flow, efficiency, etc.

Step 4

- Press the generate button for the generation of the output parameters.

Step 5

- Results are generated which include the parameters like Height of the reactor, Diameter of the reactor, Superficial air velocity, Fuel consumption rate, etc.

Step 6

- The results are printed for further design and simulation.

Step 7

- End the process.

Fig 6.10: Steps to be followed by a user

to develop a gasification modular simulation model

6.6.6.4 CODING IN VISUAL BASIC

```
*RatnadipRJoshiGasifier*
Dim a, b, c, d, e, f, g, h, i, j, k, l, m, n, o, p, q, r, s, t, u, v, w, x, y, z, a1, a3, a4 As Double

Private Sub Combo1_Click()
Text5.Text = ""
Text7.Text = ""
Text8.Text = ""
Text9.Text = ""
Text10.Text = ""
Text11.Text = ""
Text12.Text = ""
Text13.Text = ""
Text14.Text = ""
Text2.Text = CStr(Combo1.ItemData(Combo1.ListIndex))
Text4.Text = 0.25
MsgBox ("Input The Required Parameters & Generate ")
End Sub

Private Sub Command1_Click()
a = Val(Text12.Text)
b = Val(Text1.Text)
c = Val(Text14.Text)
d = (a * b) / c
Text5.Text = d

d = Val(Text5.Text)
e = Val(Text2.Text)
f = Val(Text7.Text)
```

```
g = d / (e * (f / 100))
Text8.Text = g
h = Val(Text12.Text)
i = 2.5
j = h * i
Text13.Text = j

k = 1.27
l = Val(Text8.Text)
p = Val(Text15.Text)
n = Sqr((k * l) / p)
Text11.Text = n

o = Val(Text14.Text)
p = Val(Text15.Text)
q = Val(Text6.Text)
r = (o * p) / q
Text9.Text = r

r = Val(Text9.Text)
n = Val(Text11.Text)
s = 3.14 * ((n / 2) ^ 2) * r
Text10.Text = s

x = Val(Text11.Text)
y = x / 3
Text18.Text = y

z = Val(Text4.Text)
g = Val(Text8.Text)
a1 = Val(Text19.Text)
a3 = (z * g * a1) / 1.25
```

```
Text16.Text = a3

a3 = Val(Text16.Text)
n = Val(Text11.Text)
a4 = (4 * a3) / (n ^ 2)
Text17.Text = a4
End Sub

Private Sub Form_Load()
Combo1.AddItem "Anthracite Coal"
   Combo1.ItemData(Combo1.NewIndex) = 7300
Combo1.AddItem "Bituminous Coal"
   Combo1.ItemData(Combo1.NewIndex) = 7700
Combo1.AddItem "Lignite Coal"
   Combo1.ItemData(Combo1.NewIndex) = 3892
Combo1.AddItem "Naphtha"
   Combo1.ItemData(Combo1.NewIndex) = 10984
Combo1.AddItem "Wood Chips"
   Combo1.ItemData(Combo1.NewIndex) = 5180
Combo1.AddItem "Rise Husk"
   Combo1.ItemData(Combo1.NewIndex) = 3040
End Sub

Private Sub Text1_Change()
If Text1.Text = 7760 Then
Text3.Text = 1360
End If
If Text1.Text = 5750 Then
Text3.Text = 1340
End If
If Text1.Text = 3340 Then
Text3.Text = 1240
```

```
End If
If Text1.Text = 11084 Then
Text3.Text = 10100
End If
If Text1.Text = 4300 Then
Text3.Text = 1290
End If
If Text1.Text = 1910 Then
Text3.Text = 1270
End If
End Sub

Private Sub Text2_Change()
If Text2.Text = 7300 Then
Text1.Text = 7760
End If
If Text2.Text = 7700 Then
Text1.Text = 5750
End If
If Text2.Text = 3892 Then
Text1.Text = 3340
End If
If Text2.Text = 10984 Then
Text1.Text = 11084
End If
If Text2.Text = 5180 Then
Text1.Text = 4300
End If
If Text2.Text = 3040 Then
Text1.Text = 1910
End If
End Sub
```

```
Private Sub Text3_Change()
If Text3.Text = 1360 Then
Text6.Text = 850
End If
If Text3.Text = 1340 Then
Text6.Text = 720
End If
If Text3.Text = 1240 Then
Text6.Text = 680
End If
If Text3.Text = 10100 Then
Text6.Text = 780
End If
```

6.6.7 Development of Biomass Gasifier for design Case

Design of gasifier is presented here for wood as fuel for the biomass gasifier. Calculations are also performed for following fuels and are used data for our user model development:

1) Anthracite Coal, 2) Bituminous Coal, 3) Lignite Coal, 4) Rice Husk, 5) Wood chips, 6) Naphtha

6.6.7.1 Design Statement

Following calculations are preformed for the design of a wood based biomass gasifier:

a) What is the energy needed to gasify fuel where 20 kg of wood needs to be gasified within 4 hour.
b) What is the amount of fuel needed per hour for a wood gasification system? Assume a system efficiency of 65%.
c) Find the diameter and height of the reactor, if Specific Gasification Rate of 110 kg/m^2 hr.

d) Find the time required to consume wood and amount of air needed for gasification.
e) Find the superficial velocity of air while air flow and reactor diameter is calculated. .

Solution:

Given:

Specific energy = 4300 kcal/kg

Heating value / Calorific value = 5180 kcal/kg

Density of fuel = 750 kg/m^3

Density of air = 1.25 Kg/m^3

Calorific value of producer gas = 1290 kcal/kg

Equivalent ratio = 0.25

Specific Gasification Rate = 110 kg/m^{2}hr

Stoichiometric air per kg of fuel = 3 kg air per kg of fuel

6.6.7.2 Design Parameters for Wood Chips

The energy required is:

$$Qn = \frac{20 \text{ x } 4300}{4\ hrs} \quad .$$

Q$_n$ = 21500 Kcal/hr

Fuel Consumption rate:

$$FCR = \frac{21500}{5180 \text{ x } 0.65}$$

FCR = 6.3855 kg/hr

Reactor Diameter:

$$\mathrm{D} = \frac{\{\ 1.27 \text{ X } 6.3855\ \}^{0.5}}{110}$$

Diameter =0.2715 m or 271 mm

Reactor Height:

$$\mathrm{H} = \frac{110 \text{ x } 4}{750}$$

Height = 0.5866 m or 586 mm

Time to consume wood:

$$\mathrm{T} = \frac{750 \text{ x Vr}}{750}$$

V_r = Volume of the reactor (π r^2 h)

V_r = 0.03395 m^3

$$\mathrm{T} = \frac{750 \text{ x } 0.03395}{6.3855}$$

Time = 3.98 hr

Amount of air needed for gasification:

$$\mathrm{AFR} = \frac{0.25 \text{ x } 6.3855 \text{ x } 3}{1.25}$$

AFR = 3.8313 m^3/hr

Superficial Gas Velocity:

$$\mathrm{Vs} = \frac{4 \text{ x } 3.8313}{(0.2715)^2}$$

Superficial air velocity (V_s) = 207.875 m/hr

Throat diameter ($D_{t)}$:

$$\mathrm{Dt} = \frac{27152}{3}$$

D_t = 0.9050 m

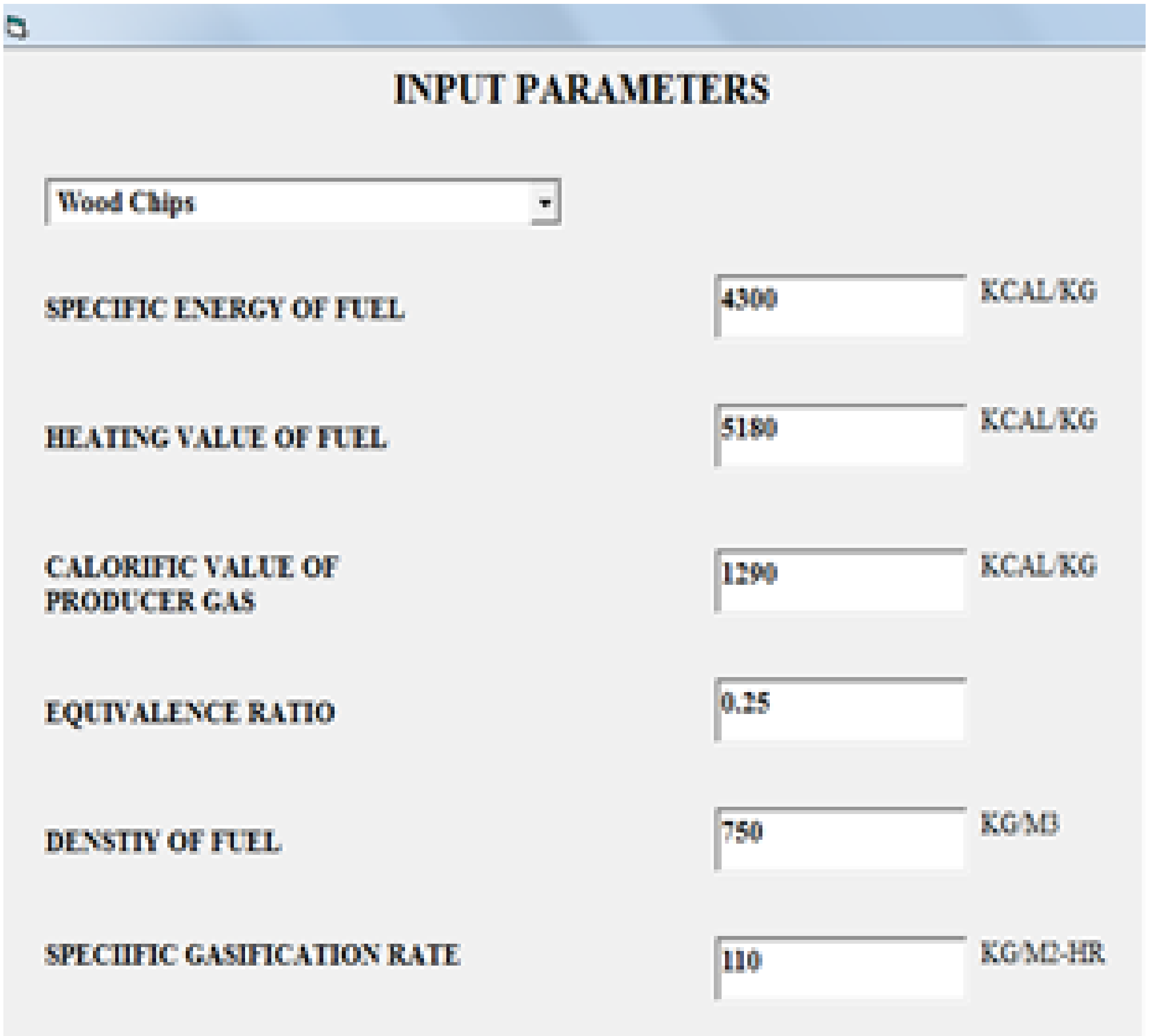
6.6.7.3 Design of gasifier with wood as fuel in Visual Basic

a) Select the fuel from the selection parameters and this case it is wood.

b) When the fuel is selected the parameters such as;

- Specific energy of fuel,
- Heating value of fuel,
- Calorific value of producer gas
- Density of fuel
- Specific gasification rate

c) Values of these parameters are already fed to the simulation model. These values are recalled while calculating the design parameters of a particular fuel. User is not required to input these data. This is the advantage of the present model built.



INPUT PARAMETERS

Wood Chips

SPECIFIC ENERGY OF FUEL	4300	KCAL/KG
HEATING VALUE OF FUEL	5180	KCAL/KG
CALORIFIC VALUE OF PRODUCER GAS	1290	KCAL/KG
EQUIVALENCE RATIO	0.25	
DENSTIY OF FUEL	750	KG/M3
SPECIIFIC GASIFICATION RATE	110	KG/M2-HR

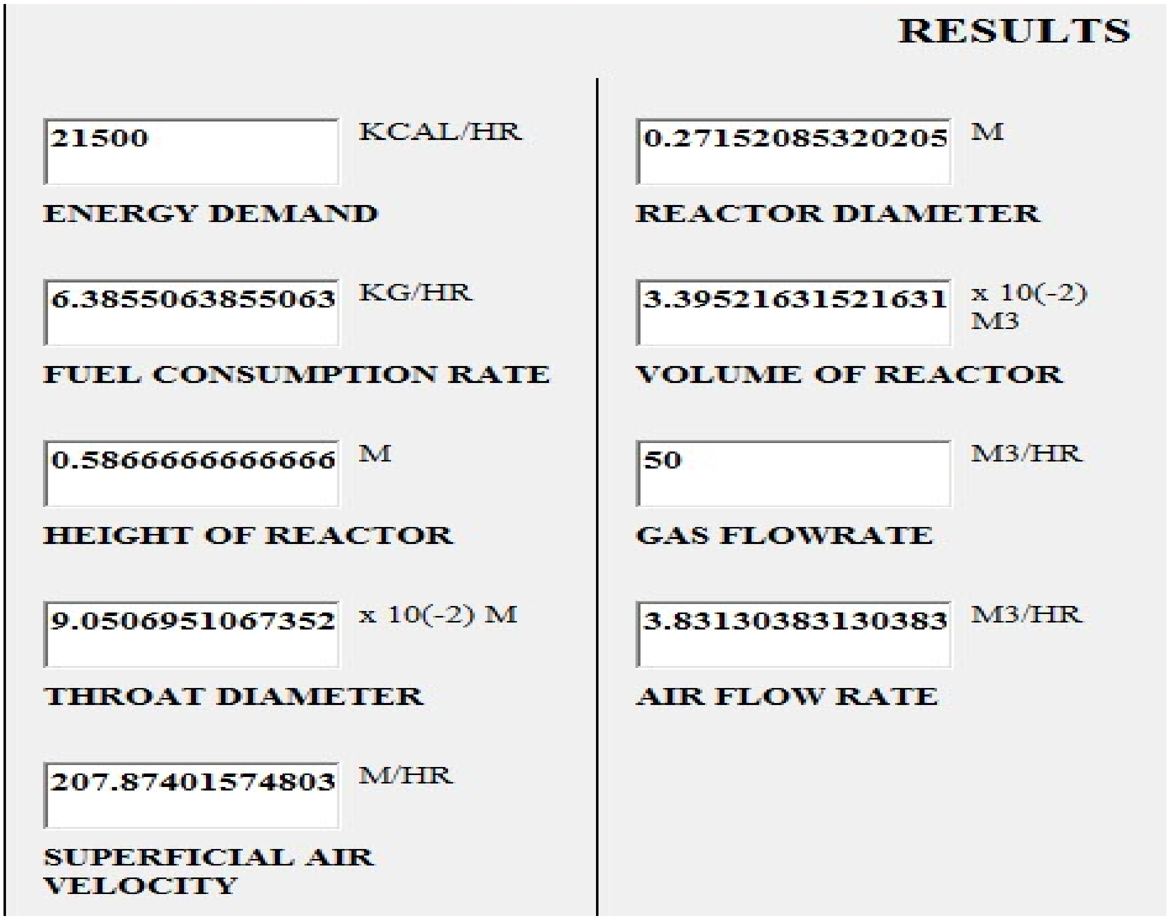
Fig 6.11: Input Parameters for wood

d) The user model will require parameters such as,

- Time for gasification
- Mass of the feed

e) The results from this design model are:

- Height of the reactor
- Diameter of the reactor
- Volume of the reactor
- Superficial air velocity
- Air flow rate
- Fuel consumption rate
- Gas flow rate
- Throat diameter



RESULTS

ENERGY DEMAND: 21500 KCAL/HR

FUEL CONSUMPTION RATE: 6.3855063855063 KG/HR

HEIGHT OF REACTOR: 0.5866666666666 M

THROAT DIAMETER: 9.0506951067352 x 10(-2) M

SUPERFICIAL AIR VELOCITY: 207.87401574803 M/HR

REACTOR DIAMETER: 0.27152085320205 M

VOLUME OF REACTOR: 3.39521631521631 x 10(-2) M3

GAS FLOWRATE: 50 M3/HR

AIR FLOW RATE: 3.83130383130383 M3/HR

Fig 6.12: Output parameters for wood gasifier

6.6.7.4 Design of gasifier with Naphtha as the fuel

Given:

Specific energy = 11084 kcal/kg.

Heating value / Calorific value = 10984 kcal/kg.

Density of fuel = 780 kg/m^3.

Density of air = 1.25 Kg/m^3.

Calorific value of producer gas = 1290 kcal/kg.

Equivalent ratio = 0.25.

Specific Gasification Rate = 190 kg/m^{2}hr.

Stoichiometric air per kg of fuel = 15 kg air per kg of fuel

Therefore the energy required is:

$$Qn = \frac{20 \text{ x } 11084}{5\ hrs}$$

$\mathbf{Q_n}$ = 44336 kcal/hr

Fuel Consumption rate:

$$FCR = \frac{44336}{10984 \text{ x } 0.65}$$

FCR = 6.209 kg/hr

Reactor Diameter:

$$\mathrm{D} = \frac{\{\ 1.27 \text{ X } 6.209\ \}^{0.5}}{190}$$

Diameter =0.203 m or 203 mm

Reactor Height:

$$\mathrm{H} = \frac{110 \text{ x } 5}{780}$$

Height = 1.217 m or 1217 mm

Time to consume wood:

$$\mathrm{T} = \frac{780 \text{ x } \mathrm{Vr}}{\mathrm{FCR}}$$

V_r = Volume of the reactor (π r^2 h)

V_r = 0.039684 m^3

$$\mathrm{T} = \frac{780 \text{ x } 0.039684}{6.209}$$

Time = 4.987 hrs

Amount Of air needed for gasification:

$$\mathrm{AFR} = \frac{0.25 \text{ x } 6.209 \text{ x } 15}{1.25}$$

AFR = 18.629 m^3/hr

Superficial Gas Velocity:

$$\mathrm{Vs} = \frac{4 \text{ x } 18.629}{(0.203)^2}$$

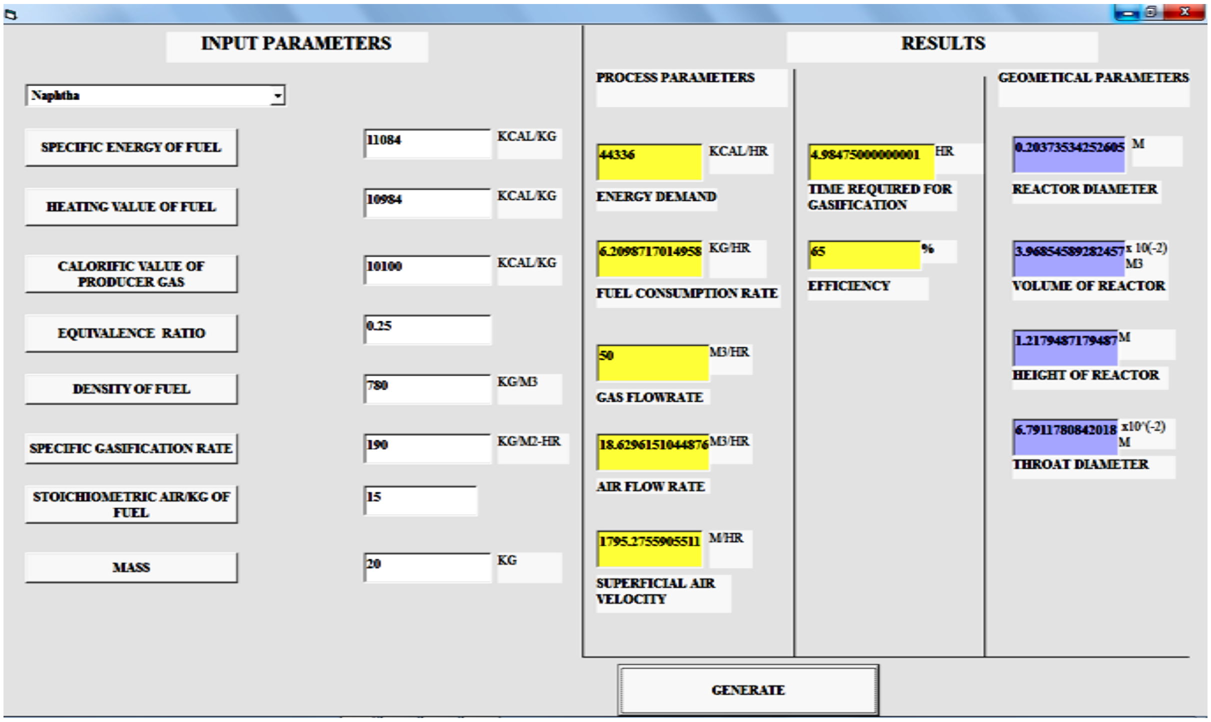
Superficial air velocity (V_s) = 1795.27m/hr

Throat diameter ($D_{t)}$:

$$\mathrm{Dt} = \frac{0.2037}{15}$$

Throat Diameter (D_t)= 0.0138 m

6.6.7.5 Design of gasifier with naphtha as a fuel



Naphtha

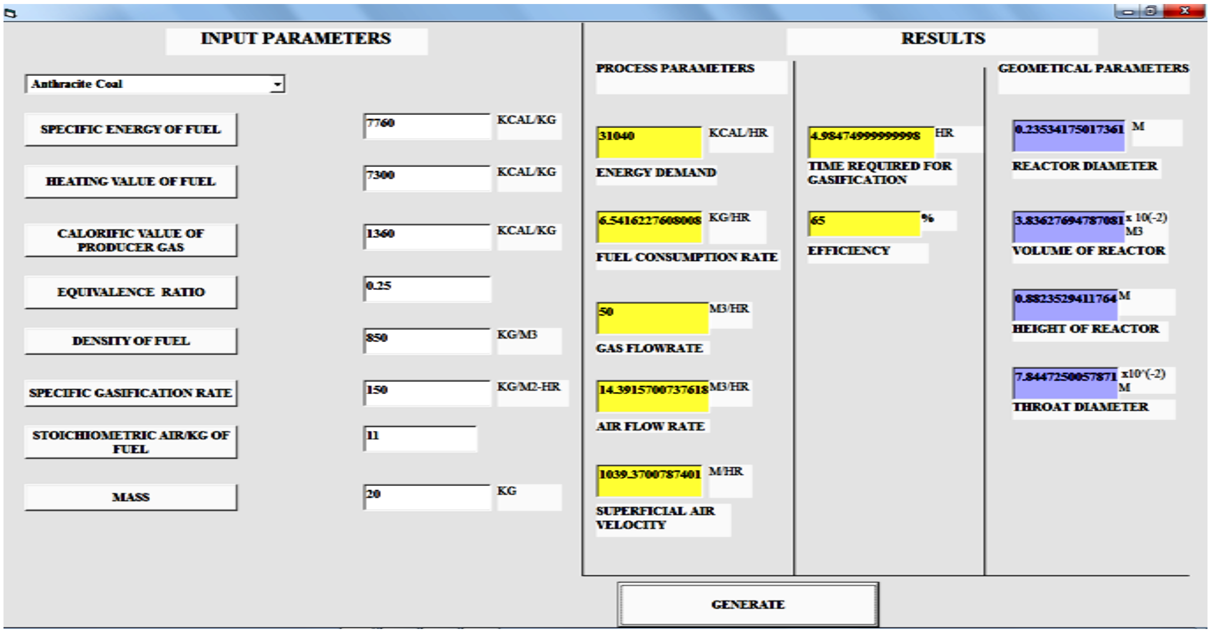
SPECIFIC ENERGY OF FUEL	11084	KCAL/KG
HEATING VALUE OF FUEL	10984	KCAL/KG
CALORIFIC VALUE OF PRODUCER GAS	10100	KCAL/KG
EQUIVALENCE RATIO	0.25	
DENSITY OF FUEL	780	KG/M3
SPECIFIC GASIFICATION RATE	190	KG/M2-HR
STOICHIOMETRIC AIR/KG OF FUEL	15	
MASS	20	KG

ENERGY DEMAND	44336	KCAL/HR
FUEL CONSUMPTION RATE	6.2098717014958	KG/HR
GAS FLOWRATE	50	M3/HR
AIR FLOW RATE	18.6296151044876	M3/HR
SUPERFICIAL AIR VELOCITY	1795.2755905511	M/HR
TIME REQUIRED FOR GASIFICATION	4.98475000000001	HR
EFFICIENCY	65	%
REACTOR DIAMETER	0.20373534252605	M
VOLUME OF REACTOR	3.96854589282457	x 10(-2) M3
HEIGHT OF REACTOR	1.2179487179487	M
THROAT DIAMETER	6.7911780842018	x10^(-2) M

Fig 6.13: Design of a naphtha gasifier

Similarly the design is carried out for various fuels and the desired output for the various fuel inputs are shown below in figures 6.14 through 6.17.

6.6.7.6 Design of a gasifier with Anthracite coal as fuel



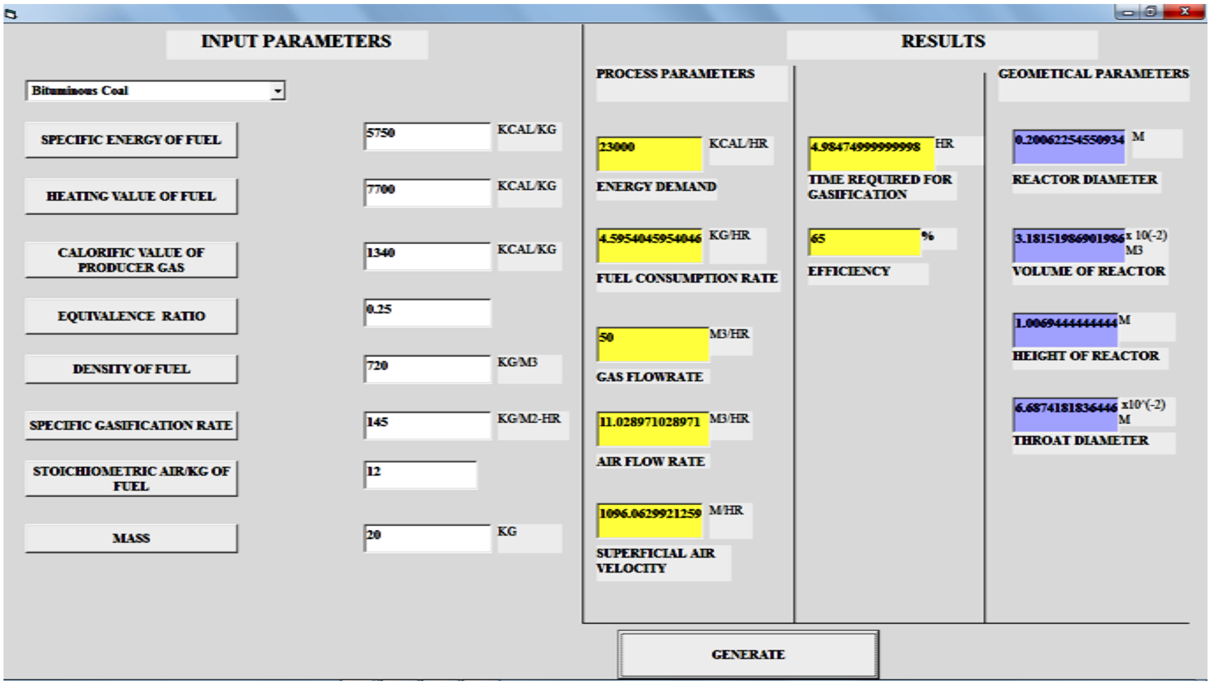
Anthracite Coal

SPECIFIC ENERGY OF FUEL	7760	KCAL/KG
HEATING VALUE OF FUEL	7300	KCAL/KG
CALORIFIC VALUE OF PRODUCER GAS	1360	KCAL/KG
EQUIVALENCE RATIO	0.25	
DENSITY OF FUEL	850	KG/M3
SPECIFIC GASIFICATION RATE	150	KG/M2-HR
STOICHIOMETRIC AIR/KG OF FUEL	11	
MASS	20	KG

ENERGY DEMAND	31040	KCAL/HR
FUEL CONSUMPTION RATE	6.5416227608008	KG/HR
GAS FLOWRATE	50	M3/HR
AIR FLOW RATE	14.3915700737618	M3/HR
SUPERFICIAL AIR VELOCITY	1039.3700787401	M/HR
TIME REQUIRED FOR GASIFICATION	4.98474999999998	HR
EFFICIENCY	65	%
REACTOR DIAMETER	0.23534175017361	M
VOLUME OF REACTOR	3.83627694787081	x 10(-2) M3
HEIGHT OF REACTOR	0.8823529411764	M
THROAT DIAMETER	7.8447250057871	x10^(-2) M

Fig 6.14: Design of an anthracite coal gasifier

6.6.7.7 Design of a gasifier with Bituminous coal as fuel


INPUT PARAMETERS

Bituminous Coal

SPECIFIC ENERGY OF FUEL	5750	KCAL/KG
HEATING VALUE OF FUEL	7700	KCAL/KG
CALORIFIC VALUE OF PRODUCER GAS	1340	KCAL/KG
EQUIVALENCE RATIO	0.25	
DENSITY OF FUEL	720	KG/M3
SPECIFIC GASIFICATION RATE	145	KG/M2-HR
STOICHIOMETRIC AIR/KG OF FUEL	12	
MASS	20	KG

RESULTS

PROCESS PARAMETERS

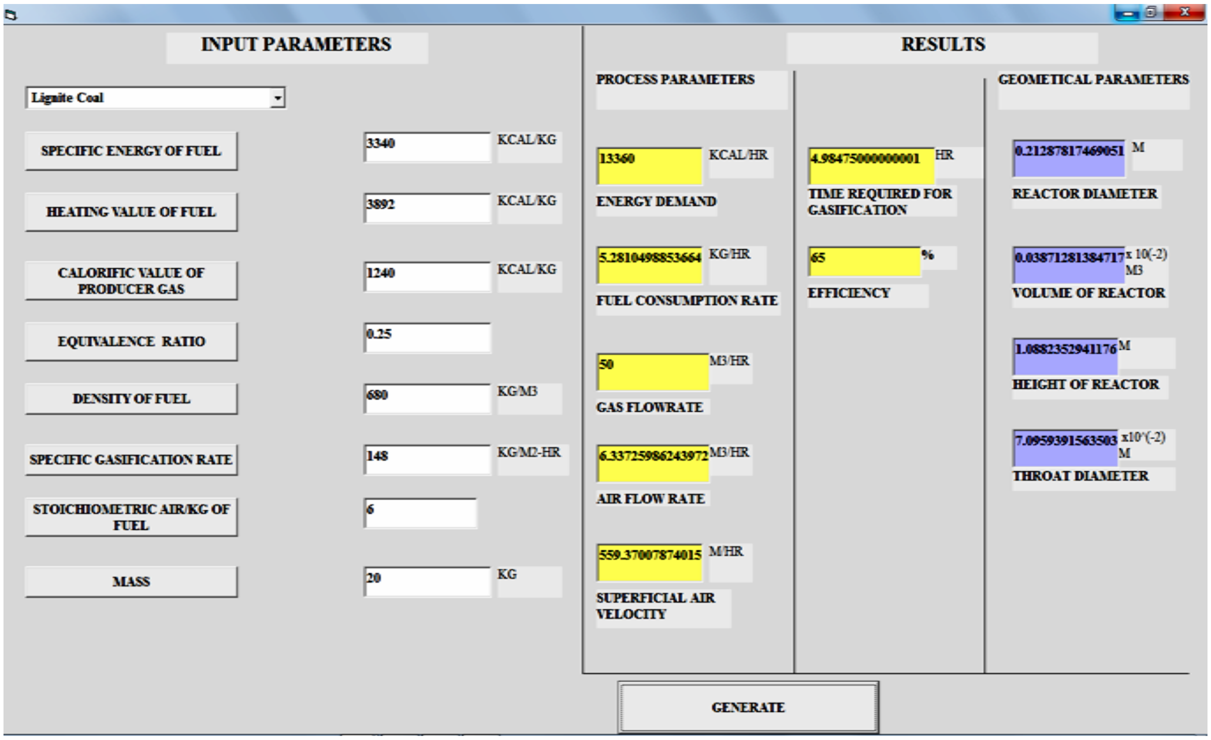
ENERGY DEMAND	23000	KCAL/HR
FUEL CONSUMPTION RATE	4.5954045954046	KG/HR
GAS FLOWRATE	50	M3/HR
AIR FLOW RATE	11.028971028971	M3/HR
SUPERFICIAL AIR VELOCITY	1096.0629921259	M/HR
TIME REQUIRED FOR GASIFICATION	4.98474999999998	HR
EFFICIENCY	65	%

GEOMETICAL PARAMETERS

REACTOR DIAMETER	0.20062254550934	M
VOLUME OF REACTOR	3.18151986901986	x 10(-2) M3
HEIGHT OF REACTOR	1.00694444444444	M
THROAT DIAMETER	6.68741818836446	x10^(-2) M

Fig 6.15: Design of a bituminous coal gasifier

6.6.7.8 Design of a gasifier with Lignite coal as fuel


INPUT PARAMETERS

Lignite Coal

SPECIFIC ENERGY OF FUEL	3340	KCAL/KG
HEATING VALUE OF FUEL	3892	KCAL/KG
CALORIFIC VALUE OF PRODUCER GAS	1240	KCAL/KG
EQUIVALENCE RATIO	0.25	
DENSITY OF FUEL	680	KG/M3
SPECIFIC GASIFICATION RATE	148	KG/M2-HR
STOICHIOMETRIC AIR/KG OF FUEL	6	
MASS	20	KG

RESULTS

PROCESS PARAMETERS

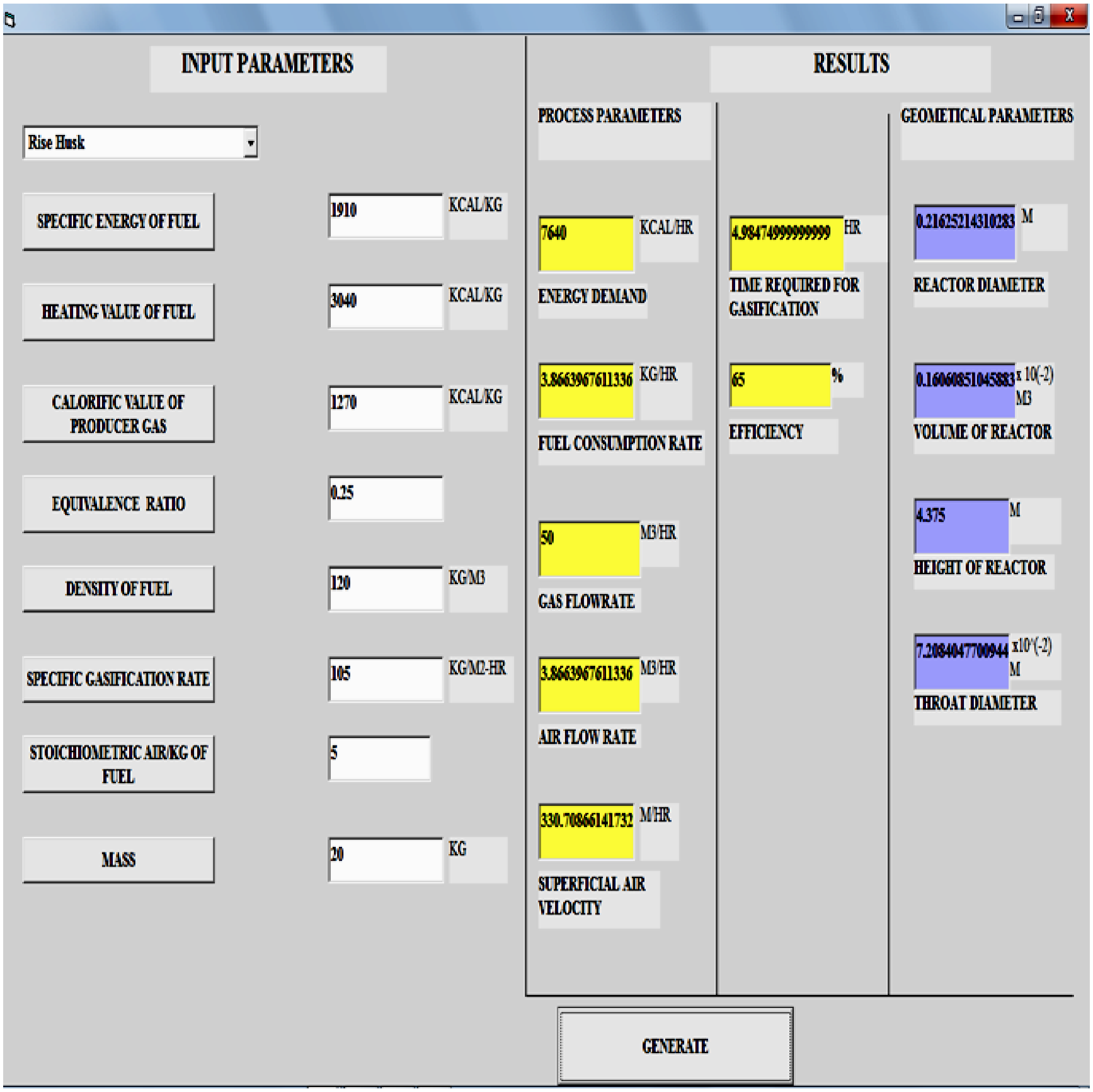
ENERGY DEMAND	13360	KCAL/HR
FUEL CONSUMPTION RATE	5.2810498853664	KG/HR
GAS FLOWRATE	50	M3/HR
AIR FLOW RATE	6.33725986243972	M3/HR
SUPERFICIAL AIR VELOCITY	559.37007874015	M/HR
TIME REQUIRED FOR GASIFICATION	4.98475000000001	HR
EFFICIENCY	65	%

GEOMETICAL PARAMETERS

REACTOR DIAMETER	0.21287817469051	M
VOLUME OF REACTOR	0.03871281384717	x 10(-2) M3
HEIGHT OF REACTOR	1.08823529411176	M
THROAT DIAMETER	7.09593915635503	x10^(-2) M

Fig 6.16: Design of a lignite coal gasifier

6.6.7.9 Design of gasifier with Rice husk as fuel



Rise Husk

SPECIFIC ENERGY OF FUEL 1910 KCAL/KG

HEATING VALUE OF FUEL 3040 KCAL/KG

CALORIFIC VALUE OF PRODUCER GAS 1270 KCAL/KG

EQUIVALENCE RATIO 0.25

DENSITY OF FUEL 120 KG/M3

SPECIFIC GASIFICATION RATE 105 KG/M2-HR

STOICHIOMETRIC AIR/KG OF FUEL 5

MASS 20 KG

ENERGY DEMAND 7640 KCAL/HR

FUEL CONSUMPTION RATE 3.8663967611336 KG/HR

GAS FLOWRATE 50 M3/HR

AIR FLOW RATE 3.8663967611336 M3/HR

SUPERFICIAL AIR VELOCITY 330.70866141732 M/HR

TIME REQUIRED FOR GASIFICATION 4.98474999999999 HR

EFFICIENCY 65 %

REACTOR DIAMETER 0.21625214310283 M

VOLUME OF REACTOR 0.16060851045883 x 10(-2) M3

HEIGHT OF REACTOR 4.375 M

THROAT DIAMETER 7.2084047700944 x10^(-2) M

Fig 6.17: Design of a rice husk gasifier

The designs of gasifiers are carried out with different fuels as feed to the gasifier. This user model is limited to use air as the medium for gasification process. This design in visual basic provides information for simulation/design using software such as HTRI, AutoCAD, HYSYS, etc.

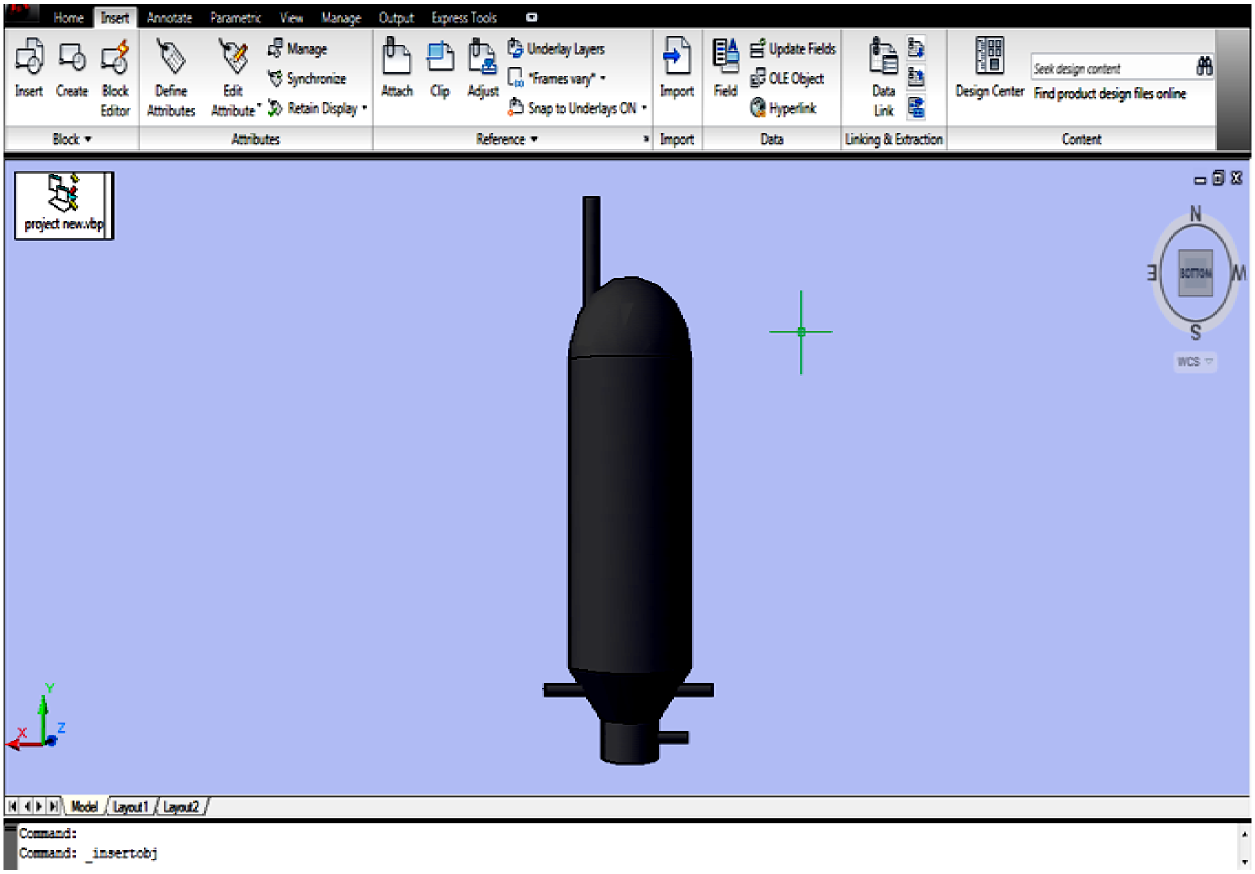
6.6.8 GEOMETRY DESIGN USING Autodesk's AutoCAD®

The visual basic programme is linked to AutoCAD such that, when values of geometrical parameters are calculated in the visual basic programme, the values of design changes in AutoCAD.

This linking is the tricky part of the embedding procedure. These two distinct software are linked with the common parameters (diameter of reactor, throat, height, etc) by coding. The parameters are named such that the value appearing in the VB platform are recalled by the AutoCAD software. In AutoCAD, linking and extraction tab allows the user to link between these two CAPE-OPEN programmes.

Generally, such modeling can be done easily and time efficiently in MS-Excel and other design tools. To tap the specific advantages of being user friendly and optimum user interface, Visual Basic as frontend is chosen for the present study.

The study now completes the full design cycle including thermodynamic and kinetic analysis, detailed process design and industry level scaled-up hydrodynamic design.



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Command:
Command: _insertobj
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Fig 6.18: Geometric design of a biomass gasifier in AutoCAD 2010

CONCLUSIONS

Based on the importance and promising nature of the gasification of biomass, modeling and simulation has been performed for finding the optimum parameters of the process.

In the present study, we have simulated full gas turbine section with optimization of biomass gasification process using Aspen HYSYS® Gibbs reactors and expander as turbine models. Although many attempts have been made to generate steam using biomass gasification process, the present investigation suggests that conditioned biomass generated fuel gas can be directly used in the gas turbine to produce enhanced power output. It is clearly seen that, due to gasifier efficiency enhancement, more H_2 is generated and this has helped to treat the fuel gas almost close to that obtained from coal gasification process. We have also carried out studies to augment the capacity of the plant and study the effect of biomass variation and size on the performance of the reactors as well as on the efficiency of the total biomass fuelled gas power plant.

A user friendly modular simulation model is developed using popular front end programming language Visual Basic. Data for calculations is provided through back end from MS-SQL. The model is also further embedded into AutoCAD to generate mechanical design parameters. Advantage earned through this embedding is industry scale-up facility generated. The present design can now be used at any scale as of requirement of a chemical process plant.

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THESIS AT A GLANCE

OVERALL CONCLUSIONS

A complete overview of energy analysis, enhancement in present real power plants with design constraints, improvisation in conventional gasifiers, innovative design of horizontal feeder gasifier, newer approach of combined feed usage for reducing single fuel dependency, and large scale efficient system development using biomass as non conventional and renewable energy resources are the salient features of the present study. These aspects touch to almost all walks of energy scenario as well as needs of society. An effort is made to provide solutions on all such difficulties converting them into opportunities with viable and rigid suggestions using modern and advanced simulation tools. By virtue of the simulating capacities of such simulation and optimization tools, various results are derived and are presented in this thesis.

A summary of work done in present thesis and their outcomes are presented below.

THESIS AT A GLANCE

Sl. No.	Topic title and contents	Conclusions/ Achievements	Page Numbers
01	**Simulation Techniques and Energy Security** • Need of simulation and optimization • Energy sector: presence and future • Energy Challenge In India	• India needs to realize the vast potential of renewable energy. • India should aim to attain a target of having 70% renewable energy use by 2050. • Brief introduction about design, modeling, simulation and optimization of chemical processes along with simulation tool Aspen HYSYS®. • Need of a reform and restructuring of the energy sector to develop globally competitive, efficient and environmentally compatible operations. • Necessity of adoption of clean coal technologies and utilization of lower-cost imported coal for coastal power plants.	1-35
02	**Enhanced Modeling and Integrated Simulation of Power Plant for Capacity Enhancement and Clean Power Production** • Thermodynamic approach • Model of Power Plant • Natural gas based	➢ Retrofitting of an existing power plant designed to produce 100 MW of power but actually producing only 93 MW power due to limitations in process design and availability of raw material feed. ➢ Simulations were carried out for 12 gas samples for different fuel supplies to redesign the fuel gas, flare gas and diesel oil systems.	36-68

	power plants ➢ Simulation of a full gas turbine (GT) ➢ Optimization for enhanced power generation	➢ By implementing the design considerations, process plant provides higher power generation (131 MW) along with omission of heating skid and incorporation of an additional gas turbine. ➢ Maximum possible power generation in four GTGs is approximately 131 MW. The existing power plant could produce only 93 MW with 31 MW each for three GTGs. ➢ Pressure control valves have been modified to accommodate the full gas flow required due to addition of one more GTG. ➢ The gasifier efficiency is enhanced using lumping parameter models for reactions by maintaining inlet temperature below 1500 ^{o}C.	
03	**Modeling, Design and Simulation of Fluidized Bed Coal Gasifier** • Coal Gasification Technologies • Gasifier Configurations • Fluidization • Mass and Energy Balance • Optimization: MATLAB code	• Many existing fluidized bed gasifiers are providing H_2/CO ratio ranging from 0.6 to 1.2, whereas our present calculations show accomplishment of 1.46. • This good quality Synthesis gas can be used as an intermediate in the production of Synthetic natural gas (SNG), ammonia and methanol. • Shell and tube heat exchanger is designed using HTRI$^{®}$ for heat recovery system. • With design calculations, it is found that the effect of coal quality becomes an unimportant parameter. Hence, the model developed and used in the	69-138

		present study becomes robust for any type of coal for medium to high capacity plants. This is an important observation considering variety and scarcity of coal in India. • From the present study, the coal density emerges as a prominent parameter affecting required height of fluidized bed.	
04	**Design and Optimization of Horizontal Feeder Gasifier** • Innovative Design to Overcome Lower Combustion Efficiencies • Design of Horizontal Feeder Gasifier • Screw Conveyor as Horizontal Feeder • Screw Conveyor Design Procedure • Optimization of the Process	❖ Innovative design of Horizontal feeder gasifier is used to reduce the limitations of direct feed injection mechanism. ❖ Horizontal feeder gasifier increases the retention time which will help to increase the reaction conversion and reactor efficiency. ❖ Enhancement of H_2/CO ratio to 3 is a major achievement of the present study. ❖ Simulation and optimization study using ASPEN HYSYS was performed considering a coal sample using its proximate and ultimate analysis and the effects of various operating parameters were studied on the product gas composition. ❖ Operating temperature of the gasifier should be 1290 K to 1330 K. This gives minimum CO_2 production along with appreciable low CO/H_2 ratio, meaning high quality of synthesis gas. ❖ It is observed that H_2 formation is increased initially and then gets dripped off as the temperature increases. CO and H_2O formation	139-187

		increases as the temperature increases. ❖ Synthesis gas production increases with the coal flow rate. ❖ As the steam rate increases mole fraction of CO decreases and hydrogen increases. ❖ The effect of oxygen flow rate was studied on product gas composition. The composition of H_2 decreases with very small deviation. The composition of CO and H_2O increases with increase in the oxygen rate.	
05	**Simulation and Optimization of Combined feed IGCC Power Plants** • Thermodynamic study • Simulation studies on various combinations of fuel feed for turbine: ➢ Syngas from Coal Gasification. ➢ Syngas from Coal and Biomass Gasification. ➢ Combined feed from Coal gasification and Naphtha. ➢ Combined feed - Coal and Natural gas	➢ This chapter elaborates another innovative approach to resolve the difficulty of power plants arising due to scarcity of one type of fuel and reduce their dependency on specific fuels. ➢ Optimization studies are carried out to see effect of various parameters on IGCC power plant using syngas from coal gasification and natural gas blending. ➢ As the pressure drop across gas turbine increases, the power generated in gas turbine also increases. ➢ As temperature of fuel gas increases, the H_2 to CO ratio decreases. But at lower temperatures, the power production is affected. ➢ As fuel gas temperature and to mixer pressure increases, the power produced increases.	188-246

		➢ Optimum value of temperature of fuel gas is taken as 900 to 1500 ^{o}C. ➢ The ratio of coal and natural gas flow rates vs power produced graph shows that; - As the ratio increases power generated increases - As natural gas flow rate increases the power generated increases ➢ There is a linear relation between oxygen flow rate and power produced. Hence, proper oxygen supply for combustion is essential. ➢ The power plant rated for 1 MW power generation is now producing 1.21 MW power. This is the success of the present work and outcome of the optimization study.	
06	**Optimization of Gas Turbine Operated on Biomass Gasification Process** - Benefits of Biomass - Power Generation - Hydrogen from Biomass - Model of the Power Plant - Simulation of a Full Gas Turbine (GT) - Gasification User	- A simulation study using Aspen HYSYS$^{®}$ software tool has been carried out to arrive at the biomass derived power output of a gas turbine under various conditions as well as to perform changes in the fuel gas system for its augmentation. - Although many attempts have been made to generate steam using biomass gasification process, the present investigation suggests that conditioned biomass generated fuel gas can be directly used in the gas turbine to produce enhanced power output.	247-297

	Model Development using Visual Basic and AutoCAD	• The simulation also shows that we could enhance the gasifier efficiency to 59% from 45 % by maintaining inlet temperature below 1500^{o}C. • Higher efficiencies help to complete conversion of CO and NOx, which in turn reduces pollution and makes this a process of clean power production. • As no data for the considered biomass at large scale is available, a comparison is made with fuel gas of coal gasification output. The results prove that the present work provides opportunities to use the biomass generated fuel gas for power generation as a safe substitute to coal gasification process. • As the standard commercial simulators do not have specified gasifiers for biomass gasification system, it was decided to develop an indigenous modular simulation which will have our design specification criteria along with our own voluminous data as back end. • A user friendly modular simulation model is developed using popular front end programming language Visual Basic. Data for calculations is provided through back end from MS-SQL. The model is also further embedded into AutoCAD to generate mechanical design parameters.	