CFD STUDY OF COAL GASIFICATION USING THAR COAL SPECIFICATIONS

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Abstract

Thar coal field is the 6th largest coal deposit in the world with an energy value greater than the oil reserves of KSA and Iran put together. A major problem in the economic growth in the country is the shortage of power and the ever increasing cost of the available power. The main reason behind this is the dependence on expensive imported fuel. The second main reason is the wrong energy mix of Pakistan. Neighboring countries like China and India and other growing economies are using coal as the main fuel to produce electricity. For economic stability and decreasing dependence on imports the energy mix has to change and most of the power plants have to be retrofitted to use coal as primary fuel.

Coal present in the Thar coal field is Bituminous coal and of low calorific value. It also contains a lot of moisture which makes it even more difficult to burn directly. Mining coal and transporting it to other locations will be expensive so a process called gasification is suggested for the coal which converts the coal into a combustible gas. This process gas can be transported to far off locations through pipelines.

A coal gasification CFD simulation model is presented in the report using the coal specification of Thar coal. The gasifier used is slurry feed type entrained flow gasifier similar to that used by Liu et al. Injections are used under the discrete phase model to define the coal entrance volumetric reactions under species transport to define the chemical reactions in the gasification process.

The detailed results study the amount of formation of all species and also the composition of product gas. The reaction rates are also studied which show the location as well as rate of reaction. Through coal gasification Pakistan will be able to harness the coal present in huge amounts in the Thar coal field.

Chapter 1

Introduction

Fossil fuels are vital sources of energy, namely, Oil, Natural Gas and Coal are the primary sources of energy and electricity in the world. These non-renewable sources, formed by anaerobic decomposition of large quantities of millions year-old dead organisms within the earth are a priceless treasure for the earth inhabitants. Fossil fuels have been used very rapidly over the past century which has given rise to environmental concerns. Fossil fuels contain high levels of carbon, ranging from volatile materials like methane which has a low carbon: hydrogen ratio, to liquid petroleum, to non-volatile substances having almost a purely Carbon ratio, such as Anthracite coal. Burning of fossil fuels produces CO2 which is a greenhouse gas. CO2 helps the atmosphere retain the energy coming from the Sun and this causes a rise in the average temperature of the Earth. This rise in temperature causes a chain adverse environmental effect which can eventually destroy the ecosystem on Earth. To avoid these adverse effects on the ecosystem alternates have been worked out to replace the existing fossil fuels being used around the world.

The renewable sources of energy are sources that are naturally replenished with at least the speed with which they are being used. Renewable energy sources consist of wind energy, solar energy, ocean energy (wave and tide), hydel-power, biofuels, geothermal energy etc. but their worldwide consumption amounted to only 13.1% (2009) [4]. All these sources have negligible effect on the atmosphere over a long period of time. The renewable energy sources are not limited by geography and are utilizable over large regions unlike the conventional fossil fuel availability. Development of new renewable energy sources lessens the dependence on conventional fossil fuels which are available in a few countries. This can help in the decrease in the import of fossil fuels which will help the economic condition of the country and also decrease the dependence on other countries for energy and power needs. Pakistan is highly dependent on the import of crude oil which has had strong effects on the economy and has at times paralyzed the budget allocated for its energy needs. Some projects of renewable energy have been established in Pakistan. These projects include the FFC Energy Ltd Wind Farm that provides about 50 MW of electricity at full load. Another project is The Quaid-e-Azam Solar Park in Bahawalpur. These projects are large scale and involve a very high capital cost. The FFC Energy Ltd project cost about 133 Million Dollars. The high capital cost of renewable energy projects have taken them out of budget of conventional power projects. Another problem with some of the renewable energy sources is that they are not dependable and provide energy with breaks. Solar energy depends upon the Sun and does not give the required output in cloudy and dusty weather. Similarly wind energy depends upon the constant blowing of wind which in turn is dependent on the weather and season. Due to all these reasons there is compromise that has to be made between the use of renewable energy projects and fossil fuel power projects. There is a need to balance the cost of energy and also install power projects that meet the energy demand of the country as well as are economically and environmentally viable.

There is also an effort to improve the efficiency of conventional fossil fuel power plants so that the consumption of fuel is reduced for the same amount of electricity. There has been a lot of work on the improvement of efficiency and different techniques have been developed to reuse waste energy and minimize losses. Devices such as economizer, reheater, heat recovery steam generator and breaking up into stages give significant improvement of efficiency. Improved boiler and gasturbine designs have also helped conserve energy which reduces the impact of the power plant on the environment.

Coal is a fossil fuel that has been used for power production by a lot of countries and is one of the cheapest to harvest depending on the location of the mines and method of extraction. About 14% of electricity produced over the world is through coal fired power plants. India and China as neighboring countries of Pakistan produce almost 70% and 80% respectively of electricity through coal. In Pakistan the electricity generation through coal is less than 1% and this is a paradox because one of the largest coal deposits in the world is present in Pakistan.A comparison of energy mix of Pakistan and that of the World is given in fig.1. Coal will replace oil as the major fuel used to produce electricity in the next 2 decades.

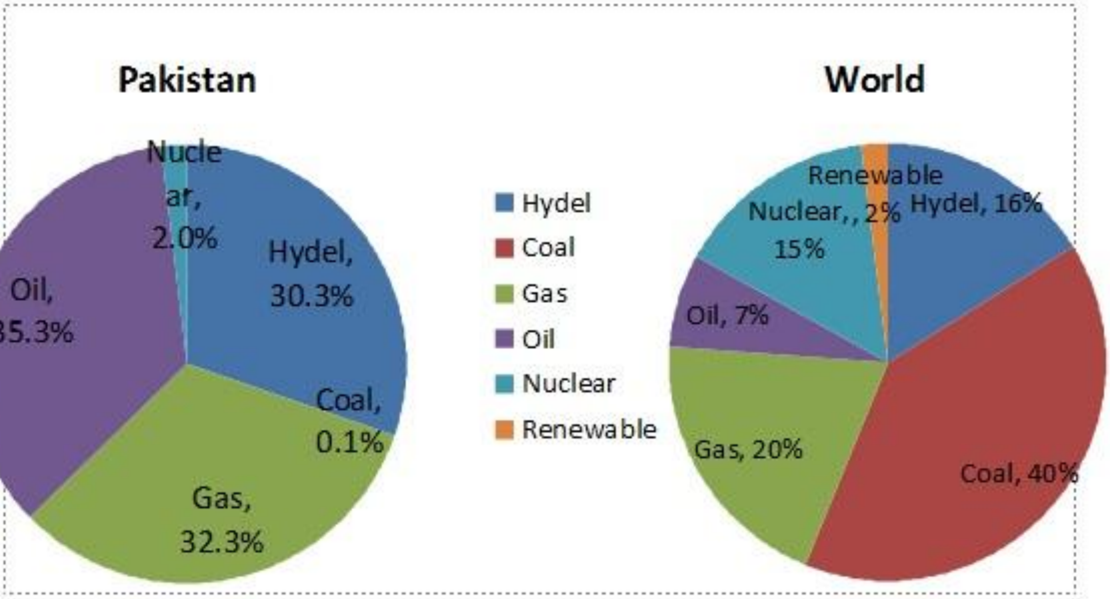


Fig.1

Pakistan is a country plighted byeconomic problems. Rapidly growing population which is already the sixth largest in the world does not have an economic growth to match it. The major problem and hurdle in the economic growth is the shortage of electric power in the country. The shortage of electricity has caused significant losses to industries which causes a decrease in exports and with closing down of factories a loss of jobs too. The load shedding is causing a 2% decrease in GDP for Pakistan.

A major problem in the load shedding is the energy mix of power plants. Most power plants are using furnace oil and/or natural gas for production of electricity. Natural gas is available at a low cost but the supply is limited to the plant has to be switched to Diesel or furnace oil to continue the production of electricity. These fuels are as much as 4 times more expensive than natural gas and the electricity produced is very expensive. This puts a load on the government and the power industry that are subsidizing the electricity being supplied to domestic and industrial customers. Recently the interest in coal has been on the rise and BQPS-1 is being converted to coal fired power plant. The coal for this plant is being imported from Malaysia. The interest in coal is due to its lower cost as compared to diesel and furnace oil. It is still 1.5 time more expensive than natural gas but provides a better and more reliable energy mix and also a lower cost of power production. The Thar coal reserves can prove to be a great hit with all these coal power plants as the coal availability will not be dependent on international relations and the available coal will be a lot cheaper than already cost effective imported coal.

Coal is considered the dirtiest fossil fuels available for burning. The salts and ash present in the coal form smoke which damages the environment and also affects the people living around the area. In recent years the research has also been focused on making coal usage cleaner and safer for the environment. Clean coal technologies have and are being developed to increase the safe usage of coal.

Clean coal technologies are the new generation methods of extracting energy from coal with marked decrease in emissions. Clean coal technologies are getting popular with increasing environmental concerns specifically over the coal fired power plants. Coal emissions are much more as compared to other fossil fuels primarily due to presence of different impurities and minerals that form ash and consequently emissions in the form of thick smoke. Study over decades has proven these emissions to cause smog, acid rain and also damage the ozone layer. Clean coal technologies result in cleaner emissions making coal fired power plants environmentally more feasible.

The first clean coal power plant was started up in September 2008 in Spremberg, Germany[1]. It was setup by a German company Siemens and owned by a Swedish company named Vattenfall. The power plant does not release carbon dioxide. Instead it captures the CO2, cools it down and pumps it underground. This method is called the Carbon Capture and Storage (CCS) method.

There are different Clean Coal Technologies and some of them are mentioned bellow:

1- Carbon Capture and Storage (CCS)
2- Carbon Sequestration
3- Coal Washing to remove minerals
4- Flue gas scrubbing
5- Desulfurization
6- Coal Gasification

All of these methods can also be used in series to minimize environmental damage caused by burning of coal.

Coal gasification is a method by which coal is heated and converted into mixture of gases which is combustible. The gas produced after gasification is called the product gas. It has a lower calorific value than coal as about a third of energy is used up during gasification. The product gas can be easily transported over long distances through pipelines and can also be injected into gas turbines. The product gas produces no smoke on combustion and is as clean as natural gas. Coal gasification has been integrated into power plants and is called Integrated Gasification Combined Cycle (IGCC) power plants.

In this research focus is on observing the performance of coal gasification and finding out the quality of product gas being produced from the gasifier. This report will start with the literature review of the work and research that has been done in the field of coal gasification. This review comprises of the literature of experimental work, model development and numerical simulations that have been done related to gasification. After the Literature review will be an explanation of basic information about coal, its types and its usage around the world. Information about Thar coals, its reserves and the conditions prevailing in the area. Following the coal section is the coal gasification information and its history. Then the theory related to the coal gasification and also related to its numerical analysis through the software is given. A walkthrough method of the simulation of coal gasification is given through Ansys Fluent. Finally the contours of different species inside the gasifier are shown and results are discussed. A conclusion ends the report and also mentions further direction where further work can be done in this field.

Chapter 2

Literature Review

Energy utilization from coal remained an interest of researcher from early ages. A lot of research and experimental work has been undertaken by many scholars around the world. The study on the coal gasification can be broken up into 3 major subgroups

1- Numerical study
2- Lab scale experimental study
3- Commercial scale projects

Of the two coal utilization methods, the CANMET Energy Technology Centre (CETC) under the Government of Canada: Department of Natural Resources has been fully functional in investigating, progressing, and upgrading combustion and gasification technologies which also include oxy-coal combustion, which is an alternative to post- combustion capture for carbon capture and storage (CCS) and the integrated gasification combined cycle (IGCC) with CCS <CO2 capture and storage>. The CETC piloted research on the bench and pilot-scale through experiments with the capability of advanced modeling techniques which included simulations and modeling environments. The modeling capability was used to simulate oxy-coal combustion in the field and has been presented by Chui et al [1-3]. Furthermore, in China application of the modeling capability has contributed betterment in boilers to reducing greenhouse gas emissions.

In the past, there have been a small number of experimental investigations into entrained flow gasifiers, hence the data that is available is limited mostly to lab scale gasifiers, and even fewer results from pilot scale gasifier experiments. Out of the several experiments that have been performed in history, the following are mentioned. Using a lab scale oxy-coal gasifier in Brigham-Young University; Brown et al. [5] conducted such experiments as have been mentioned. They used intrusive probes for sampling, and obtained syngas and temperature composition measurements along the gasifier axis. By means of the RANS model of these gasifiers, Hill and Smoot [6] conducted CFD simulations and matched results with the experimental data. For measurement, they injected coal particles along with oxygen into the

BYU axial flow gasifier using a centralized injector, and injected steam from the concentric secondary injectors.

The Mitsubishi Heavy Industries (MHI) gasifier is an air-coal swirling flow gasifier of which they have pilot and research versions built. These are described to have fuel handling capacity of 2 tons/day and 200 tons/day, respectively. The air-blown swirling flow type gasifiers have two sections, gasification process occurs in the upper part and combustion occurs downstream. In order to make the good mixing flow in the gasifier, the combustor segment is injected with fuel particles as well as tangential air jets. In the gasification section more coal is injected. Watanabe and Otaka [7] have simulated the Mitsubishi two-stage gasifier as well as by Chen et al. [8, 9].

Similar to the reactive flows which are found in gasification, multiphase flows are mathematically modeled via two approaches. They are the (LPEF) Fluid models and (EPEF) Fluid models. In the first method, the properties of solid particles are pursued using a Lagrangian methodology, while the surrounding gas phase is replicated using Eulerian approach method. The process in each is designed through the conservation equations of energy, mass and momentum, in which the two phases are coupled through source terms. In the EPEF method, the solid phase equation is solved using the Eularian approach. The volume fraction that characterizes the volume of the solid is solved locally by an additional equation. The gas phase is also replicated by the Eularian approach. The EPEF method is more convenient that LPEF for computing the grouped influence of the particles in different regions of the reactor vessel where the solid particle volume fraction is quite large. When the flow velocities are higher than is usually found in EFGs and the particles are present throughout the flow, the LPEF method is typically used instead [11]. The LPEF method has been used in different combustion like gas turbines, diesel and petrol engines. These types of engines have fuel droplets from the injectors which are required to be tracked.

Researches on entrained flow gasifiers have RANS method and single-dimension approach. Monaghan and Ghoniem [12] used a reactor network to build a one-dimensional gasification model, which complied with previous experimental data along the entire length of the reacting vessel. EFG computations were performed by Kumar and Ghoniem [13] that ranged from research scale to the commercial scale applying RANS model in turbulence. Kumar et al. established that while k–ϵ performs well for the gasification with non-turbulent injection, k–σ has a better performance for gasifiers that have turbulence and swirling flow inside them. The study of gasification has also been carried out at the level of a single particle. Watanabe et al. [7] have used the MHI gasifier to simulate multi-dimensional RANS model in CFD.

In order to define and identify the char consumption kinetics and fuel vaporization processes different qualities of coal have been studied by Kobayahsi et al. [14] and Ubhayaker et al. [15]. Goetz et al. [16] studied the effects of char-consumption mechanism on gasification process. Katijani et al. [17] analyzed gasification char mechanism process in steam and CO_2 in a drop tube pressurized gasifier. Singer and Ghoniem [18] successfully developed models of sub-particle structure and studied their char consumption properties.

Gasifiers of various scales, including a 2 t/day bench-scale, an 8 t/day and a 200 t/day pilot-scale gasifier, were being investigated since 1980s by Japanese scientists Araki et al. in 1996; Hara et al. in 1997; Kaneko et al. in 1997. Plants of various scales are expected to be constructed and examined over the next few years, ranging up to a 1.5-2 k t/day commercial plants. For a current Japanese IGCC project Ciaxia et al. [19] developed a broad-range simulation model for entrained flow coal gasifiers.

Coal

Coal is a natural resource found within the confines of the Earth and has the potential to generate power for us. The deposits of this organic rock were formed from ancient vegetation, and are extracted from the amalgamated layers of other rock strata. Coal is found in seams which range in thickness from less than a millimeter to that of many meters.

The composition of coal is carbon (50 to 98 percent), hydrogen (2 to 13 percent) and oxygen- along with smaller volumes of nitrogen, sulphur and other elements. The rock also contains a lesser quantity of water and grains of inorganic matter turn into residual ash when coal is burnt.

Types of coal are distinguished by their color; over millions of years, and under the right conditions, the chemical and physical changes to the rock cause an increase of hardness and organic maturity; a progressive coalification from peat into anthracite results. The degree of transformation of the original plant material to carbon determines the ‘rank’ of the coal.[6]The lower the rank, the less the heat given out and moisture and ash content is high. As you go up the ranks, the higher carbon provides more heat, as well as is the cleanest coal to use. [7]

Low Ranking

High moisture, low Carbon/Energy

High in oxygen and hydrogen content

Lignite

Soft, resembles soil more than rock

Color can range from dark black to many shades of brown

Up to 45% moisture content

Used largely in electricity production

Sub-Bituminous

Electricity generation

Cement manufacturing

Other Industrial uses

Hard Coal

Low moisture, high Carbon/Energy

Low in Hydrogen and Oxygen

Bituminous

Same uses as sub-bituminous

Iron extraction and Steel manufacturing

Anthracite

Hardest

Black, lustrous color

Moisture content is less than 15%

Used domestically and industrially

Creates smokeless flame

Coal Reserves around the world

According to the "Statistical Review of World Energy" (2013), the world has reserves of 187 trillion cubic meters of natural gas, 861 billion tonnes of coal, and 1669 billion barrels of crude oil.

Crude Oil and Natural gas are expected to have 53 and 56 years of extraction remaining, respectively.

Coal on the other hand, holds enough proven world reserves to last 109 years.[3]

These figures slightly change over the years according to world consumption patterns, and the number scan be increased by the discovery of further fossil fuel reserves.

Proven world reserves are those which have been explored and found viable for extraction using the available mining technologies. Many more reserves may lie in wait, for governmental policies and exploratory groups to invest in extraction and (development) projects for their fields. Such is the case of the Thar coal field in Pakistan.

Worldwide Usage of Primary Energy Sources

The energy consumption of the world is predicted to increase more than 50 percent over the coming thirty years- while all nations that are rapidly developing will be increasing their usage of coal to cope up with the increasing energy needs.

Although oil has been the primary energy source, the trend is rapidly changing. More than half of the world’s coal usage was tallied to China in 2012, for the first time. Both India and China remarkably increased their coal consumption by 6.1% and 9.9%, respectively, and they will likely make it their main energy resource in the upcoming decades. The IEA predicts that coal will most definitely replace oil as the primary fuel used to produce electricity by year 2017. [9]

Emerging economies accounted for 80% of the global increase in energy consumption. As one of these emerging economies, Pakistan’s energy demand is also rapidly rising for the sake of industrialization and development. With industrialization, rising incomes and higher per capita energy for a population which is set to surpass 190 million by 2015, indeed adds up to higher energy demand. As a result, the total primary energy supply in the country is expected to quadruple by 2025. The state of power generation in the country, however, clangs alarm bells for us.

The currently installed energy generation capacity is 17,897 MW and the projected demand was 24,400 MW in 2010. That demand is expected to triple or quadruple by 2025, eventually causing a gap of 95,798 MW between currently installed capacity and the projected demand. There is a mojr economic impact due to this energy deficit. Firms which have installed private generating plants and those which have not, are losing billions of rupees per year, along with a loss of industrial employment accounting for 300,000 jobless people. [10]

Load-shedding has resulted in 157 billion RS loss to industries, 219 billion RS loss to economy, costing 2% of GDP, 75 billion RS loss if exports, and loss of 400000 employees- all due to load shedding. (Source: BH National University Publications- Emerging from the Energy Crisis-2008)

The un-self-sufficiency of power production in Pakistan is burdening the nation's shoulders and implying serious economic and development threat to the people. Even more so, future years predict a never ending flux of financial deficit due to import costs, loans and a vicious cycle of poverty.

A solution is provided with the exploration of the Thar coal project. It will help Pakistan meet its energy shortages and is very important for the energy security of Pakistan.

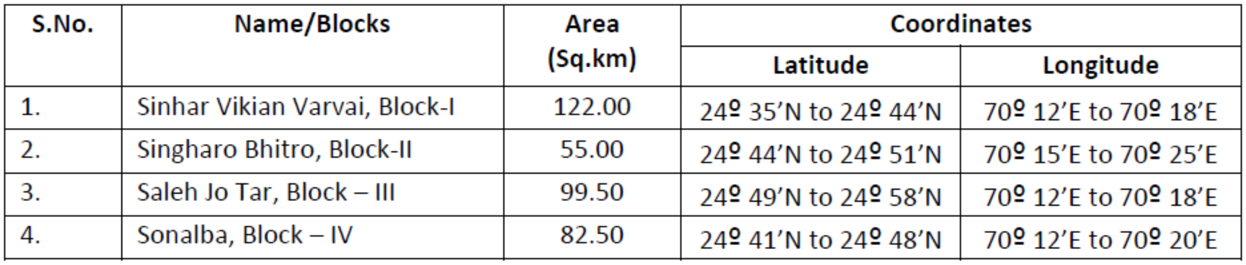
95850 GWh POWER was PRODUCED in Pakistan during 2005-2006. Oil, gas and hydel take the majority of the cake at around 30% each. Imported furnace oil sources, and other imported fuel sources, hydel power, nuclear, renewable, gas, whereas there was next to no production via coal.[10]

Through coal exploitation, Pakistan will be able to step in to the self-sustainable league and put an end to the many threats facing the country.

Chapter 3

Thar Coalfield

The Thar coalfield location is between the Latitudes 24ºN and25ºN and Longitudes 69ºE and 70ºE in lower part of Sindh Province. GSP selected four blocks considering their ease for exploration and assessment of coal resources. The blocks with their respective details are given in Table-1[10]:



S.No.	Name/Blocks	Area (Sq.km)	Coordinates	
			Latitude	Longitude
1.	Sinhar Vikian Varvai, Block-I	122.00	24º 35'N to 24º 44'N	70º 12'E to 70º 18'E
2.	Singharo Bhitro, Block-II	55.00	24º 44'N to 24º 51'N	70º 15'E to 70º 25'E
3.	Saleh Jo Tar, Block – III	99.50	24º 49'N to 24º 58'N	70º 12'E to 70º 18'E
4.	Sonalba, Block – IV	82.50	24º 41'N to 24º 48'N	70º 12'E to 70º 20'E

Table-1

Islamkot is at a distance of about 400 km away from Karachi. The railway line is up to Naokot, which is nearly 100 km from that mines area.

Relief, Topography and Climate

Thar coalfield is located in the Thar Desert which is one of the largest deserts in the world. Thar region varies between near sea level to more than a hundred and fifty meters above sea level.

The climate is arid to semi-arid with intense dry and hot summers and relatively cold and dry winters. It is one of the most densely populated deserts of the world with a population more than 90 thousand. The people are totally reliant on livestock and very little agriculture.

Water Resources

There is very little rainfall in this part of the desert with a very dry weather. Water bodies present in whatever limited amount are of prodigious worth to the population and livestock.

Rain water collects in depressions and water holes. These water holes consist of silt mud and caliche material.

There is underground water also present varying in different areas. Studies show the presence of three possible aquifer zones at varying depths some are above the coal zone some are within the coal zone and some are below it.

Geology

Thar coalfields are covered with sand dunes up to a depth of eighty meters and rests upon a structural platform in the eastern part of the desert. It comprises of 3 parts Basement Complex, coal bearing Bara Formation, alluvial deposits and sand.

Reserves

Analysis of the Thar coal field has shown that there is an estimated 175 billion tons of coal to be mined. The evaluation of the four blocks in the region is shown in the following table.

S.No.	Name/Blocks	Area (Sq.km)	Reserves (Million Tonnes)			
			Measured	Indicated	Inferred	Total
1.	Sinhar Vikian Varvai, Block-I	122.00	620	1,918	1,028	3,566
2.	Singharo Bhitro, Block-II	55.00	640	944	-	1,584
3.	Saleh Jo Tar, Block – III	99.50	413	1,337	258	2,008
4.	Sonalba, Block – IV	82.50	684	1,711	76	2,471
Total:		358.5	2,357	5,910	1,362	9,629

Table-2[10]

Thar Coal Composition and Properties

Ash	5.2 ~ 6.5
Volatile Matter	26.5 ~ 33
Fixed Carbon	19 ~ 22
Moisture	43 ~ 49
Sulphur	1 ~ 1.3
Heating value (Btu/lb)	As Received 5780 to 6398

Table-3[10]

The above table-3[10] shows the composition of coal found in the Thar coal region. It can be easily analyzed that the coal has high moisture content and less that 50 percent consists of carbon and volatile matter that is ignitable.

Coal gasification

In a gasification process coal is heated in the absence of oxygen (or controlled amount of oxygen) and presence of steam to produce a mixture of methane, carbon monoxide, carbon monoxide and hydrogen. This mixture is combustible and dust free; however it has a lower calorific value than the unprocessed coal. The resulting coal gas can be used as fuel in gas turbines and is also easier to transport.

The industry in Pakistan is the largest consumers of natural gas. Specifically the fertilizer and power industries take the lion's share [13]. The process gas from gasified coal has proved to be very suitable for fertilizer industries and power plants.

A Brief History of Coal Gasification

Coal gasification has been used over the centuries to provide for domestic and commercial heating, lighting and cooking. Coal can be gasified in a many simple ways. The coal gasification was first discovered by Jan Baptista van Helmont (1577–1644) who was from Netherland. He discovered that by heating coal or wood a spirit was released that he named 'gas'. The first used method of gasification was to heat coal in a retort in the absence of air, partially converting coal to gas with coke as a byproduct; William Murdock a Scottish engineer was the pioneer of this method for commercial gasification of coal in 1792.

Murdock licensed his process to the Gas Light and Coke Company in 1813 and to Baltimore Gas Company in 1816 which is the first coal gasification company in the United States [14].

Coal Gasification techniques

A number of coal gasification techniques are being used or are under research around the world. Some of the techniques will be discussed here.

Underground Coal Gasification:

Underground coal gasification (UGC) is a technique used to convert underground coal in coal mines to gas using a number of boreholes. A controlled amount of a combination of oxygen and steam is injected into a gasification panel inside the coal seam. The steam heats the coal and in the presence of limited amount of oxygen a controlled reaction takes place producing a gas called "Syn Gas" which is then extracted from the coal seam.

Underground coal gasification is also a pilot project in the Thar Coal Block V. The pilot project has planned a 100 MW UGC based power plant. Renowned Scientist Dr. Samar Mubarakmand is heading this project under the Planning Commission, Government of Pakistan. It has been estimated that this project will cost about 1.8 billion rupees in the initial phase [15]. This project has also faced opposition from scientists around Pakistan in favor of open pit mining of coal.

Entrained Flow Gasification

Entrained flow gasification is a technique that can produce low emission "syn gas". Entrained Flow Gasifiers (EFG) is an important component of IGCC power plants (Integrated Gasification Combined Cycle). In the entrained flow gasification process pulverized coal and a controlled amount of oxygen are injected into a vertical chamber at high pressure and high temperature that produces a mixture of CO2, CH4, H2 and CO. Ash formed from the process and other impurities are removed from the bottom of the gasifier in the form of slag. The research work and advancement in regards to EFGs will be discussed in detail in the following sections.

Other gasification processes

There are two other commercial processes currently in use the Winkler process and the Koppers-Totzek process [14]. Oxygen steam and finely powdered coal are reacted together. A fluidized bed is used in the Winkler process in which finely powdered coal is mixed with the oxidizing gas. A very high temperature is required for the Koppers-Totzek process, the coal is entrained in the gases passing through the reactor. Ash accumulates in the form of molten slag which is removed from the lower end of the gasifier. The Koppers-Totzek process is a type of entrained flow gasification process. These processes are currently being used for fuel gas production and in the generation of gases for chemical and fertilizer production.

Chapter 4

Theory Governing the Coal Gasification

The modeling of coal gasification is governed by different occurrence that is shown in the following segments. The models used to solve the problem are also identified in each section.

Turbulence

Turbulence is the three-dimensional unsteady random motion observed in fluids at moderate to high Reynolds numbers. As technical flows are typically based on fluids of low viscosity, almost all technical flows are turbulent. Many quantities of technical interest depend on turbulence, such as:

- Mixing of momentum, energy and species
- Heat transfer
- Pressure losses and efficiency
- Forces on aerodynamic bodies

While turbulence is, in principle, described by the Navier-Stokes equations, it is not feasible in most situations to resolve the wide range of scales in time and space by Direct Numerical Simulation (DNS) as the CPU requirements would by far exceed the available computing power for any foreseeable future. For this reason, averaging procedures have to be applied to the Navier-Stokes equations to filter out all, or at least, parts of the turbulent spectrum. The most widely applied averaging procedure is Reynolds-averaging (which, for all practical purposes is time-averaging) of the equations, resulting in the Reynolds-Averaged Navier-Stokes (RANS) equations. By this process, all turbulent structures are eliminated from the flow and a smooth variation of the averaged velocity and pressure fields can be obtained. However, the averaging process introduces additional unknown terms into the transport equations (Reynolds Stresses and Fluxes) which need to be provided by suitable turbulence models (turbulence closure). The quality of the simulation can depend crucially on the selected turbulence model and it is important to make the proper model choice as well as to provide a suitable numerical grid for the selected model. An alternative to RANS are Scale-Resolving Simulation (SRS) models. With SRS methods, at least a portion of the turbulent spectrum is resolved in at least a part of the flow domain. The most well-known such method is Large Eddy Simulation (LES), but many new hybrids (models between RANS and LES) are appearing. As all SRS method require time-resolved simulations with relatively small time steps, it is important to understand that these methods are substantially more computationally expensive than RANS simulations.

To incorporate turbulence in a problem on of the following models can be used:

1. Spalart-Allmaras model
2. k-ϵ models
    - Standard k-ϵ model
    - Renormalization-group (RNG) k-ϵ model
    - Realizable k-ϵ model
3. k-ω models
    - Standard k-ω model
    - Shear-stress transport (SST) k-ω model
4. v^2 – f model (add-on)
5. Transition k-kι-ω model
6. Transition SST model
7. Reynolds stress models (RSM)
    - Linear pressure-strain RSM model
    - Quadratic pressure-strain RSM model
    - Stress-omega RSM model
8. Scale-Adaptive Simulation (SAS) model
9. Detached eddy simulation (DES) model, which includes one of the following RANS models.
    - Spalart-Allmaras RANS model
    - Realizable k-ϵ RANS model
    - SST k-ω RANS model
10. Large eddy simulation (LES) model

k-ϵ Model

The k-ϵ (2-equation) Standard model is used for the turbulence in the coal gasification process. Two-equation models are historically the most widely used turbulence models in industrial CFD. They solve two transport equations and model the Reynolds Stresses based using the Eddy Viscosity approach. The standard k-ϵ model in ANSYS FLUENT makes the cut of models and has been the mainstay of many practical engineering flows. This model was suggested by Launder and Spalding [17]. The model is very popular and often used because of its stability and economy.

The draw-back of all k-ϵ models is their insensitivity to adverse pressure gradients and boundary layer separation. They typically predict a delayed and reduced separation relative to observations. This can result in overly optimistic design evaluations for flows which separate from smooth surfaces (aerodynamic bodies, diffusers, etc.). The k-ε model is therefore not widely used in external aerodynamics.

Standard k- ϵ Model Transport Equations

k, is the turbulent kinetic energy and its rate of dissipation, ϵ, are found from the following transport equations:

$$\frac{\partial y}{\partial t}(\rho k) + \frac{\partial y}{\partial x_i}(\rho k u_i) = \frac{\partial y}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - \rho\varepsilon - Y_M + S_k$$

(1)

And

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) = \frac{\partial y}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}\left(G_k + C_{3\varepsilon}G_b - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k} + S_\varepsilon\right)$$

(2)

G_k characterizes the increase of turbulent kinetic energy k due to the changes in the speed of particles. G_b is the increase of turbulence kinetic energy by the effect of buoyancy, as shown in the k- ϵ Model. Y_M signifies the influence of the inconsistency in the expansion of compressible turbulence to the dissipation rate overall. $C_{1\epsilon}$, $C_{2\epsilon}$, $C_{3\epsilon}$ are all constants. σ_k and σ_ϵ are the Prandtl numbers for turbulence for k and ϵ, correspondingly.

Modeling of Chemical Reactions

In the model of Transport of chemical species and its mixing is done by simultaneous solution of diffusion, convection, turbulence and reaction equations for all individual species. Many chemical reactions can be modeled simultaneously, many of the reactions that are occurring in the bulk phase and also on wall or particle surfaces. The modeling aptitudes of species transport are explained.

For non-premixed systems modeling a turbulent flame, the method of reaction progress variable can be used for premixed systems, the partially premixed approach, or the composition PDF Transport.

The reactions can be classified into four types:

- Volumetric Reactions
- Wall Surface Reactions and Chemical Vapor Deposition
- Particle Surface Reactions
- Reacting Channel Model

Species Transport Method

Solving the chemical conservation equations for each component, mass fraction of each local species Y_i is forecasted through the coupled equation of convection-diffusion. The general chemical conservation equation can be presented in the following form:

$$\frac{\partial}{\partial t}(\rho Y_i) + \nabla.(\rho \vec{v} Y_i) = -\nabla.\vec{J_\iota} + R_i + S_i$$

(3)

In the above equation R_i is the average speed of species production *i* by chemical reaction and S_i is the speed of creation by dispersed phase addition plus other user-defined function. This sort of equation is solved for *N-1* species where *N* is the number of species existing in the problem. As total mass fraction of all species is 1, so the mass fraction of any specie is found out by subtracting *N-1* species mass fractions. To diminish calculation error, the highest mass fraction is selected as the *i*th species, N_2 has the highest fraction when air is taken as the oxidizing agent.

Mass Diffusion In Species Transport

In turbulent flows, the mass diffusion general equation takes the following form:

$$\vec{J_\iota} = -\left(\rho D_{i,m} + \frac{\mu_t}{S_{Ct}}\right)\nabla Y_i - D_{T,i}\frac{\nabla T}{T}$$

(4)

Where Sc_t is the Schmidt number for turbulence ($\frac{\mu_t}{\rho D_t}$) where μ_t is viscosity for turbulence and *Dt* is the diffusivity of turbulence). The default value of Sc_t is taken as 0.7. The effects of turbulence are considerably large as compared to the laminar effects so considering the laminar effects of diffusion is not necessary. This is also valid for the current problem.

Energy Equation in Species Transport

The enthalpy of transport in mixing flows due to species diffusion

$$\nabla.\left[\sum_{i=1}^{n} h_i \vec{J_i}\right]$$

can have a momentous weight on the enthalpy field and should be considered in each case. In particular, when the Lewis number

$$Le_i = \frac{k}{\rho c_p D_{i,m}}$$

(5)

for any species is far from unity, neglecting this term can lead to significant errors. This term is included by the software in the calculation by default. In Equation 005, k is the thermal conductivity.

Discrete Phase

Developments in the field of CFD have given a deeper understanding of multiphase flow dynamics. The 2 approaches employed for the solution of multiphase flows are Euler-Lagrange approach and the Euler-Euler approaches as explained in the paragraphs below:

The Euler-Lagrange approach

The model for Lagrangian discrete phase model in the software used; follows the Euler-Lagrange approach. The Navier-Stokes equations are solved by considering the fluid as a continuum, whereas the dispersed phase is elucidated by tracking a large number of particles, bubbles, or droplets through the flow field calculations. The dispersed phase can exchange momentum, mass, and energy with the fluid phase.

This approach is made considerably simpler when particle-particle interactions can be neglected, and this requires that the second phase dispersion dwell in a low volume fraction, even when high mass loading is present. The particle trajectories are calculated in the fluid phase calculation as specific intervals. The model is made suitable for the modeling of coal and liquid fuel (droplets) combustion, and some particle-laden flows, but incorrect for homogenized fluids or any application where there is a significant second phase volume fraction. For applications such as these, particle-particle interactions can be included using the Discrete Element Model, which is discussed in Discrete Element Method Collision Model.

Dense Discrete Phase Model

In the standard formulation of the Lagrangian multiphase model, the assumption is that the volume fraction of the discrete phase is sufficiently low: it is not taken into account when assembling the continuous phase equations. The general form of the conservation of mass and conservation of momentum conservation equations are given in Equation 006 and Equation 007

$$\frac{\partial y}{\partial x} + \nabla.(\rho\vec{v}) = S_{DPM} + S_{other}$$

(6)

$$\frac{\partial \rho \vec{v}}{\partial t} + \nabla . (\rho \vec{v} \vec{v}) = -\nabla p + \nabla . \tau + \rho \vec{g} + \overrightarrow{F_{DPM}} + \overrightarrow{F_{other}}$$

(7)

To overcome this limitation of the Lagrangian multiphase model, the volume fraction of the particulate phase is accounted for by extending Equation 6 and Equation 7 to the following set of equations

$$\frac{\partial}{\partial t}\left(a_p \rho_p\right) + \nabla . \left(a_p \rho_p \overrightarrow{v_p}\right) = \sum_{q=1}^{nphases} \left(\grave{m}_{qp} - \dot{m}_{pq}\right)$$

(8)

$$\begin{aligned} \frac{\partial}{\partial t}\left(a_p \rho_p \overrightarrow{v_p}\right) &+ \nabla . \left(a_p \rho_p \overrightarrow{v_p} \overrightarrow{v_p}\right) \\ &= -a_p \nabla p + \nabla . \left[a_p \mu_p \left(\nabla \overrightarrow{v_p} + \nabla \overrightarrow{v_p^T}\right)\right] + \ a_p \rho_p \vec{g} + F_{vm,lift,user} \\ &+ \sum_{q=1}^{nphases} \left(\overrightarrow{K_{qp}}\left(\overrightarrow{v_q} - \overrightarrow{v_p}\right) + \dot{m}_{qp} \overrightarrow{v_{qp}} - \dot{m}_{qp} \overrightarrow{v_{qp}}\right) + K_{DPM}\left(\vec{v}_{DPM} - \vec{v}_p\right) \\ &+ S_{DPM,explicit} \end{aligned}$$

(9)

Here, Equation 8 is the mass conservation equation for an individual phase *p* and Equation 9 is the corresponding momentum conservation equation. Currently, the momentum exchange terms (denoted by *DPM*) are considered only in the primary phase equations.

In the resulting set of equations (one continuity and one momentum conservation equation per phase), those corresponding to a discrete phase are not solved. The solution, such as volume fraction or velocity field, is taken from the Lagrangian tracking solution.

The software applies a special treatment to the particle momentum equation as soon as the particle volume fraction exceeds a certain user specified limit. Thus, the unlimited accumulation of particles is prevented. In turn, this allows the simulation suspensions and flows like bubbling fluidized bed reactors, operating at the packing limit conditions, allowing for multi disseminated particle systems. However, no Discrete Element Method (DEM) type collision treatment is applied, which would otherwise allow the efficient simulation of systems with a large number of particles.

Modeling Species Transport in Multiphase flows

Species transport is also applied to multiphase flows. To solve the chemical species multiphase flow the conservation equations for each phase *k*, the prediction of local mass fraction of each species Y_i^k, by solving convection-diffusion equation for the i^{th} species. The conservation equation for chemical species in the generalized form (3), when applied to a multiphase mixture can be represented in the following form

$$\frac{\partial}{\partial t}\left(\rho^q a^q Y_i^q\right) + \nabla.\left(\rho^q a^q \vec{v}\ \ {}^q Y_i^q\right) = -\nabla. a^q \vec{J}_i^q + a^q R_i^q + a^q S_i^q + \sum_{p=1}^{n}\left(\dot{m}_{p^i q^j} - \dot{m}_{q^i p^j}\right) + \mathcal{R}$$

(10)

Where R_i^q is the average production rate of homogeneous species *i* by chemical reaction for phase q, $m_{q}{}^{j}{}_{p}{}^{i}$ is the source of mass transfer between species i and j from phase *q* to *p*, and *R* is the reaction speed of homogeneous species. In addition, a^q is the volume fraction for phase q and S_i^q is the rate of formation by accumulation in the dispersed phase and any user-defined function source.

Chemical reactions that are homogenous in the gas phase are used the similarly as a chemical reaction in a single phase. The reactants and the products are present in the same mixture, and so they belong to the same phase. The volume fraction of the particles decides the rate of reaction of the phase in question.

Char-gas Reactions

Several types of chemical reactions are taking place inside the gasifier at high temperatures. These reactions can be classified into homogeneous and heterogeneous reactions.

Heterogeneous Char-gas reactions

The heterogeneous char-gas reactions include char-O_2, char-steam, char-H_2 and char-CO_2 reactions. The reactions are listed as following:

1- Char–O2 reaction presented by Wen and Chaung in 1979

$C + 1/2O_2 \rightarrow CO$

2- Char–steam reaction presented by Dobner in 1976
$C + H_2O \rightarrow CO + H_2$

3- Char–CO2 reaction Dutta *et al* in 1977
$C + CO_2 \rightarrow 2CO$

4- Char–hydrogen reaction Wen in 1968

$C + H_2 \rightarrow CH_4$

Homogeneous Char-gas reactions

There are also some homogeneous reactions taking place inside the gasifier. They are listed below [19]:

1- Fuel gases combustion by Siminski*et al* in 1972

$H_2 + 0.5O_2 \rightarrow H_2O$

$CO + 0.5O_2 \rightarrow CO_2$

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

2- Water–gas shift reaction presented by Singh and Saraf in 1977

$CO + H_2O \rightarrow CO_2 + H_2$

3- Methane–steam reforming reaction presented by Zahradnik and Grace in 1974

$CH_4 + H_2O \rightarrow CO + H_2$

Chapter 5

Problem Description

A coal gasifier is selected according to the dimensions of the entrained flow gasifier simulated by Xiang Jun Liu et al [19]. A two dimension model is of the gasifier is made and air inlets are adjusted according to the area ratio of the original gasifier.

The 2-D model of the gasifier along with its dimensions is given below.

2D CAD Model of Coal Gasifier

2D model given below has been made using NanoCAD 5 Commercial Version [20].

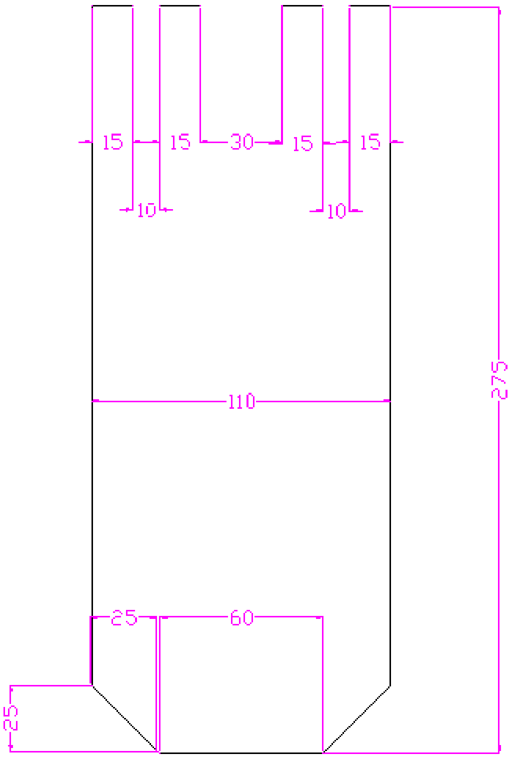


Fig. 1

The coal slurry and air enters from the top. The coal slurry enters the gasifier from the opening in the middle which is 30mm in diameter and the air enters the gasifier from the holes on each side of the coal slurry entrance, these holes are 10mm wide. The total width of the gasifier is 110mm and the total length is 275 mm.

2D Mesh of Coal Gasifier

The mesh is made using the Gambit 2.4.6 version. The details of the mesh are as follows:

Mesh Size

Level	Cells	Faces	Nodes	Partitions
0	7625	15540	7916	1

Mesh Quality

Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality.

Minimum Orthogonal Quality = 6.08148 e-01

Maximum Aspect Ratio = 4.12311 e+00

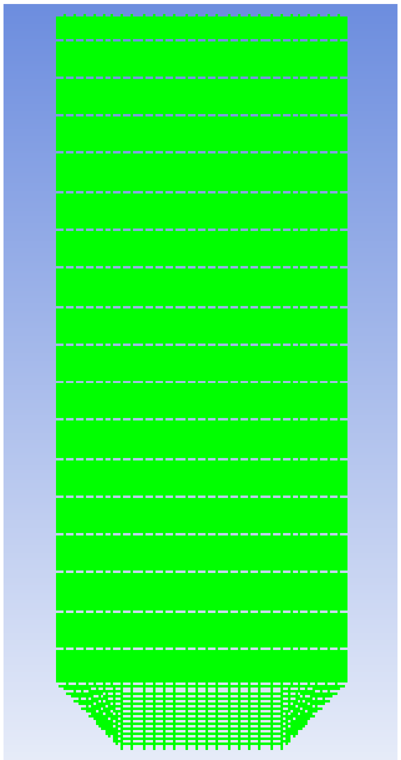


Fig. 2

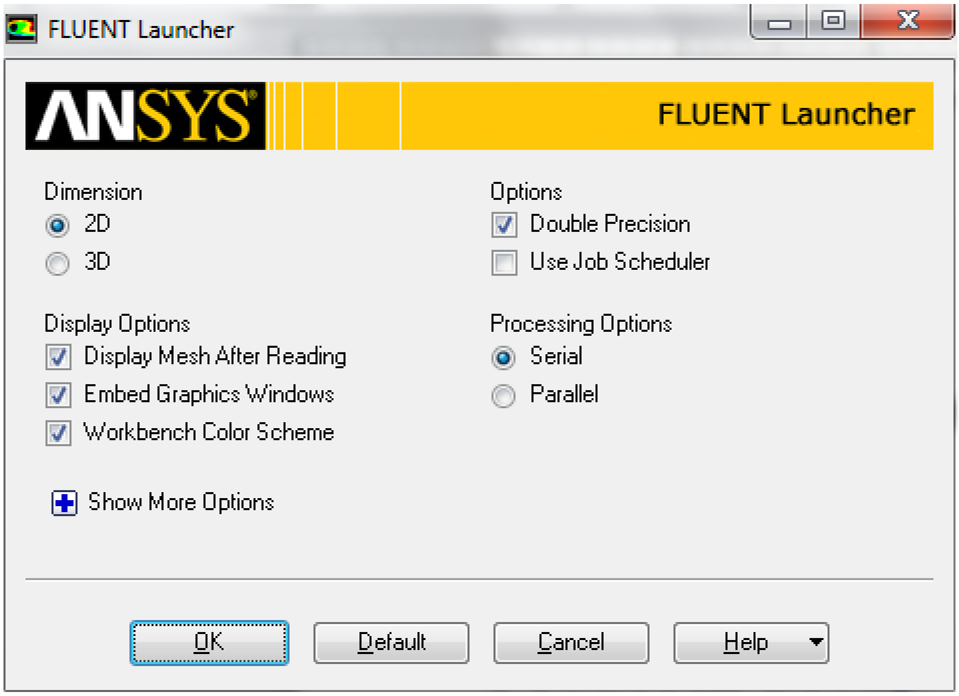
Mesh Type

The meshing is done using the Quad-Map scheme. Only the triangular region near the bottom of the mesh is through the Tri-Pave scheme.

Problem Setup

The previously mentioned coal gasifier mesh is imported into Ansys Fluent 14.0 for further pre-processing, solution and post-processing.

The options selected while opening Ansys Fluent are 2D double precession and serial processing is chosen by default. The diagram of the Ansys Fluent Launcher is shown below:



Dimension
● 2D
○ 3D

Options
☑ Double Precision
☐ Use Job Scheduler

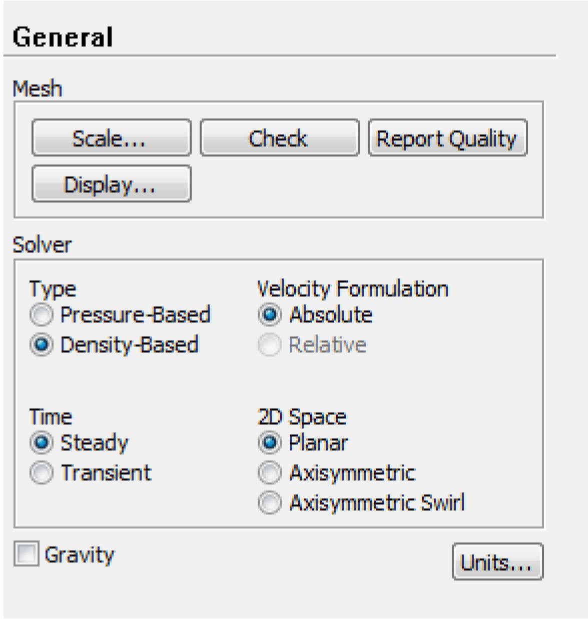
Display Options
☑ Display Mesh After Reading
☑ Embed Graphics Windows
☑ Workbench Color Scheme

Processing Options
● Serial
○ Parallel

Fig. 3

General Settings

Density-Based solver type is used because of high velocities present inside the gasifier. Steady state is selected to find the solution for steady state conditions during gasification. For the 2D mesh the settings of 2D planar are used.



Solver

Type
○ Pressure-Based
● Density-Based

Velocity Formulation
● Absolute
○ Relative

Time
● Steady
○ Transient

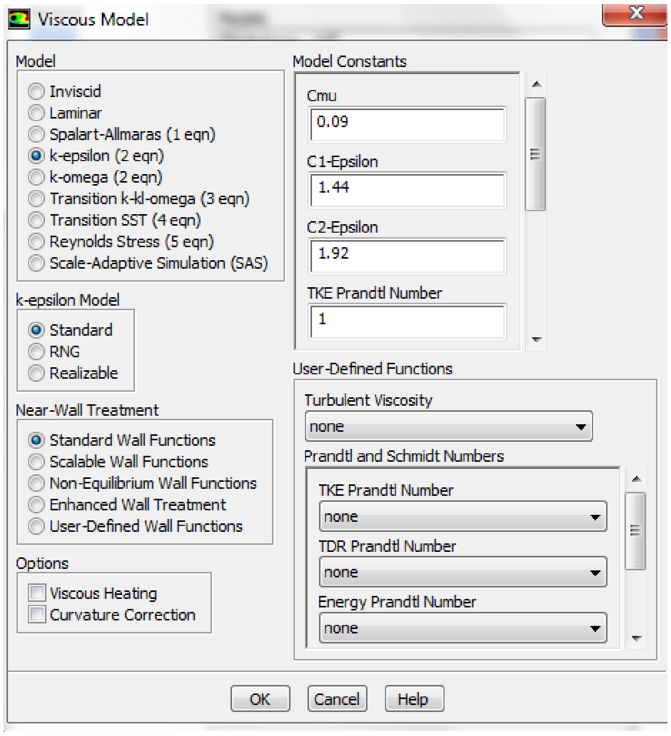
2D Space
● Planar
○ Axisymmetric
○ Axisymmetric Swirl

☐ Gravity

Fig. 4

Viscous Model

K-epsilon Standard (2 equation model) is used to define the viscosity in the problem. Other values are taken as default.



Model
○ Inviscid
○ Laminar
○ Spalart-Allmaras (1 eqn)
● k-epsilon (2 eqn)
○ k-omega (2 eqn)
○ Transition k-kl-omega (3 eqn)
○ Transition SST (4 eqn)
○ Reynolds Stress (5 eqn)
○ Scale-Adaptive Simulation (SAS)

k-epsilon Model
● Standard
○ RNG
○ Realizable

Near-Wall Treatment
● Standard Wall Functions
○ Scalable Wall Functions
○ Non-Equilibrium Wall Functions
○ Enhanced Wall Treatment
○ User-Defined Wall Functions

Options
☐ Viscous Heating
☐ Curvature Correction

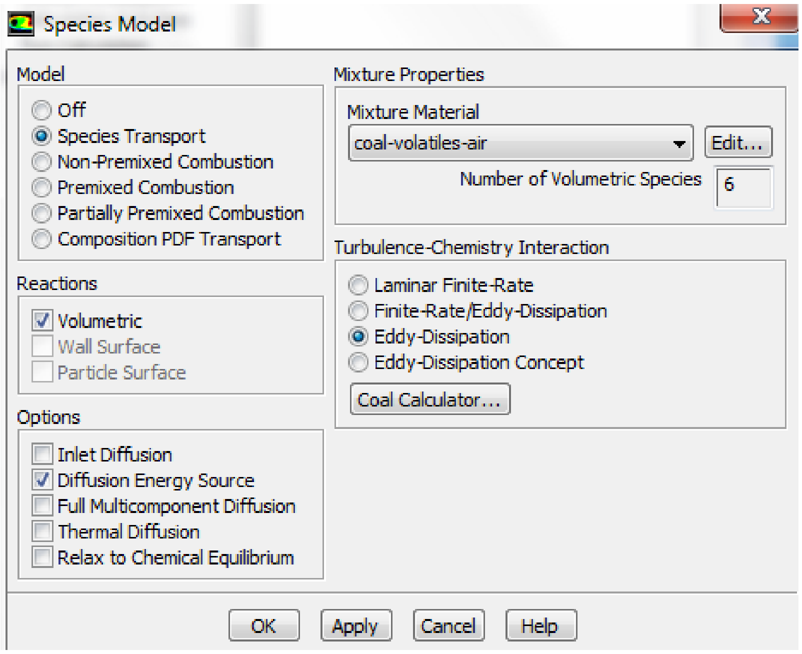
Model Constants
Cmu: 0.09
C1-Epsilon: 1.44
C2-Epsilon: 1.92
TKE Prandtl Number: 1

User-Defined Functions
Turbulent Viscosity: none
Prandtl and Schmidt Numbers
TKE Prandtl Number: none
TDR Prandtl Number: none
Energy Prandtl Number: none

Fig. 5

Species Model

Species Model deals with the chemical reactions taking place inside the gasifier. Species Transport model is employed to with volumetric reactions. Eddy-Dissipation option is selected under Turbulence-Chemistry interaction.


Species Model

Model
○ Off
● Species Transport
○ Non-Premixed Combustion
○ Premixed Combustion
○ Partially Premixed Combustion
○ Composition PDF Transport

Reactions
☑ Volumetric
☐ Wall Surface
☐ Particle Surface

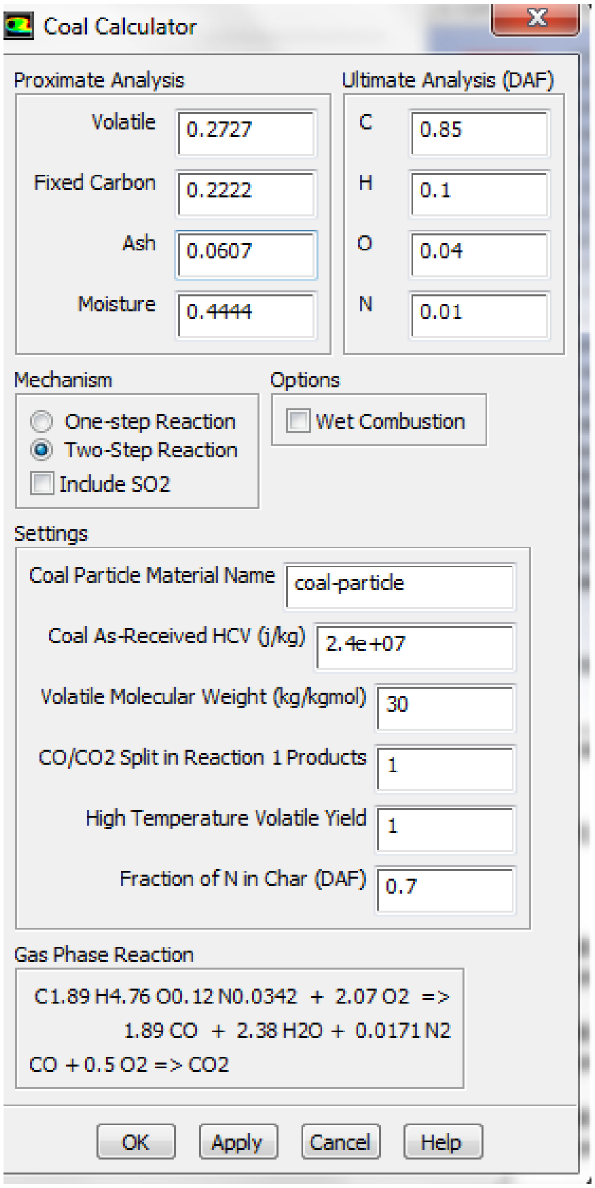
Options
☐ Inlet Diffusion
☑ Diffusion Energy Source
☐ Full Multicomponent Diffusion
☐ Thermal Diffusion
☐ Relax to Chemical Equilibrium

Mixture Properties
Mixture Material: coal-volatiles-air
Number of Volumetric Species: 6

Turbulence-Chemistry Interaction
○ Laminar Finite-Rate
○ Finite-Rate/Eddy-Dissipation
● Eddy-Dissipation
○ Eddy-Dissipation Concept

Fig. 6

The coal calculator under Turbulence-Chemistry Interaction is used to define the Proximate Analysis of coal used which in this case is Thar coal. Two step reaction is chosen which is also shown in the Gas Phase reaction panel in figure 7 below.



Proximate Analysis

Volatile 0.2727
Fixed Carbon 0.2222
Ash 0.0607
Moisture 0.4444

Ultimate Analysis (DAF)

C 0.85
H 0.1
O 0.04
N 0.01

Mechanism

○ One-step Reaction
● Two-Step Reaction
☐ Include SO2

Options

☐ Wet Combustion

Settings

Coal Particle Material Name coal-particle
Coal As-Received HCV (j/kg) 2.4e+07
Volatile Molecular Weight (kg/kgmol) 30
CO/CO2 Split in Reaction 1 Products 1
High Temperature Volatile Yield 1
Fraction of N in Char (DAF) 0.7

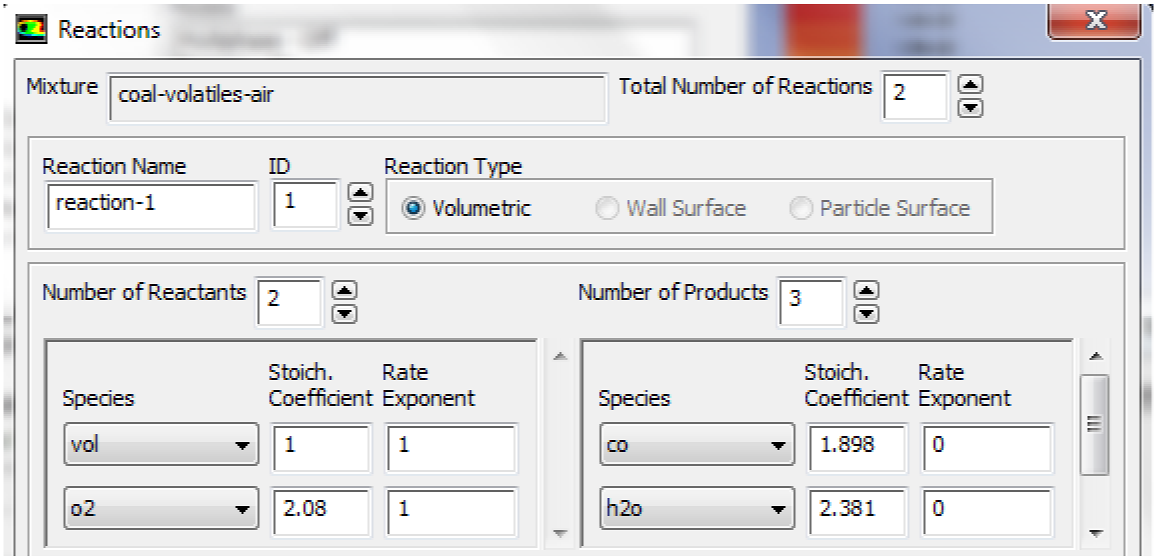
Gas Phase Reaction

$C_{1.89}H_{4.76}O_{0.12}N_{0.0342} + 2.07\,O_2 \Rightarrow 1.89\,CO + 2.38\,H_2O + 0.0171\,N_2$

$CO + 0.5\,O_2 \Rightarrow CO_2$

Fig. 7

Chemical reactions are also defined as shown in figure 6 through the edit button. A sub window opens when edit reaction is clicked. The defined reactions are shown in the following window:



Reactions

Mixture: coal-volatiles-air

Total Number of Reactions: 2

Reaction Name: reaction-1

ID: 1

Reaction Type: ● Volumetric ○ Wall Surface ○ Particle Surface

Number of Reactants: 2

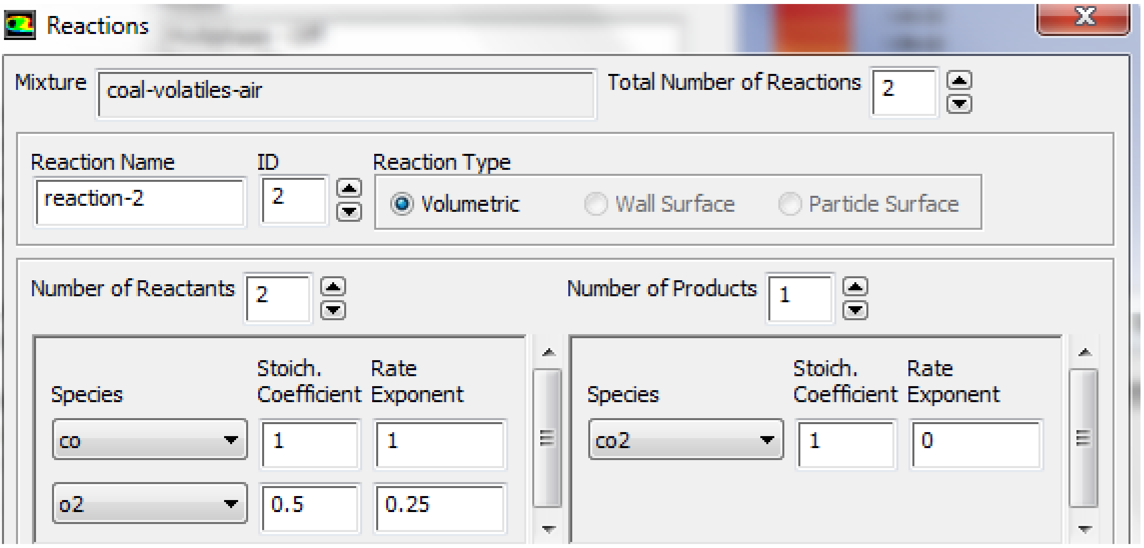
Species	Stoich. Coefficient	Rate Exponent
vol	1	1
o2	2.08	1

Number of Products: 3

Species	Stoich. Coefficient	Rate Exponent
co	1.898	0
h2o	2.381	0

Fig. 9

The following diagram shows the defining of the second reaction



Reactions

Mixture: coal-volatiles-air

Total Number of Reactions: 2

Reaction Name: reaction-2

ID: 2

Reaction Type: ● Volumetric ○ Wall Surface ○ Particle Surface

Number of Reactants: 2

Species	Stoich. Coefficient	Rate Exponent
co	1	1
o2	0.5	0.25

Number of Products: 1

Species	Stoich. Coefficient	Rate Exponent
co2	1	0

Fig. 10

The two step reaction helps in the estimation of amount of formation of carbon mono-oxide which is necessary for the purpose of this research.

Defining Materials

Materials are defined from the materials window and all species participating in the reaction and resulting as products from the reaction are defined. Additionally chemically inert gases like N2 are also defined which play no part in the reactions.

Boundary Conditions

The gasifier is a vertical body where the air and coal slurry enter from the top and the products exit from the bottom. The coal slurry enters from the center of the gasifier at low speeds and the air enters at an angle from the two sides at high speeds. This high differential of velocity causes turbulent mixing of air and coal slurry which results in better chemical reactions between the reactants. The boundary conditions are as follows:

Coal Inlet boundary conditions

Mass flow rate of coal slurry = 1.82643 kg/s = 6,575 kg/h

Inlet velocity normal to opening = 23.11 m/s

Turbulent intensity of coal slurry = 10%

The coal inlet is defined through injections under Discrete Phase Model tab. 9 injections define the inlet conditions of coal with varying particle sizes and mass flow rates for each injection.

Air Inlet boundary conditions

Air inlet velocity at 30 to the opening= 242 m/s

Turbulent intensity of air = 12%

Solution Methods

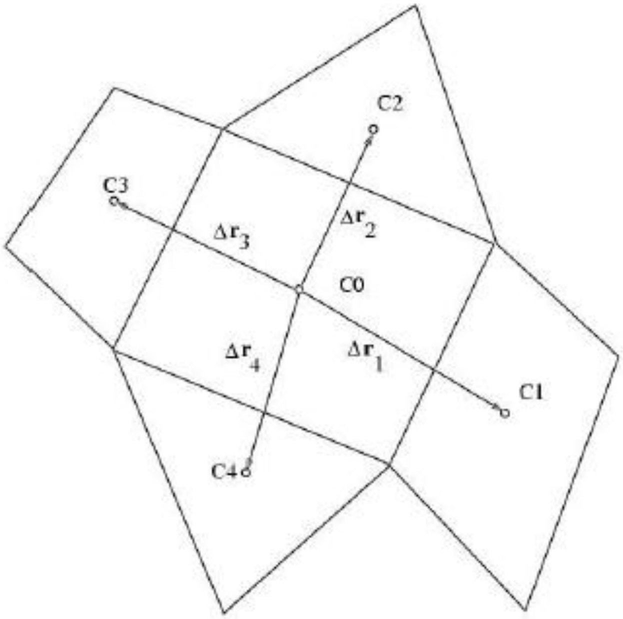
Schemes used for pressure-velocity coupling and other spatial discretizations are given as follows:

Pressure Velocity Coupling: SIMPLEC

The SIMPLEC (Semi-Implicit Method for the Pressure Linked Equations Consistent) is an algorithm proposed initially by Patankar and Spadling. This scheme is generally used for incompressible flows. The scheme has been gradually improved over time to give faster convergence and better results as compared to SIMPLE and PISO schemes. SIMPLE and SIMPLEC are almost identical and give the same corrected pressure. The only a slight difference is the way the pressure correction is calculated.

Gradient: Least Squares Cell Based

The least squares method uses the values of the neighboring cells to approximate a value assuming local linearity.



Least Squares Method

Pressure: PRESTO!

Pressure values on control volume faces are required for discretization of momentum equation. The STANDARD scheme of pressure discretization uses the cell center values on the faces for pressure interpolation. However the PRESTO! Scheme uses the values on the faces. This is done by making use of staggered grids and where pressure variables are not correlated with the velocity. The PRESTO! Scheme has a higher computational cost as it requires more memory for the staggered grids. The PRESTO! Scheme works better with flows with high swirl and turbulence.

Second Order upwind scheme:

Second order upwind is a scheme of discretization of hyperbolic equations. This is a technique which calculates values in one direction using values from the other direction. Upwind schemes are basically finite difference method that are adaptive and simulate the flow of information in the direction of fluid flow. The difference between first and second order upwind is that the second order upwind uses 3 previous points instead of 2 as in the case of first order upwind.

Momentum: Second Order upwind (First order upwind for first 100 iterations)

Turbulence: Second Order upwind (First order upwind for first 100 iterations)

Species: Second Order upwind (First order upwind for first 100 iterations)

Energy: Second Order upwind

Under Relaxation Factors

Under relaxation factors in Fluent are set at default which is suitable for most cases and is also a good option to start the iteration. If the residuals start increasing the under relaxation factors should be reduced. Reduced relaxation factors will cause the solution to reach conversion very slowly. So it is advisable to start with a larger under relaxation factor.

The default under relaxation is unsuitable for special cases where the problem involves high turbulence. Sometimes when the under relaxation factor is increased the residuals shoot up but the increase dies down over time. It is a good practice to increase the under relaxation factors after some iterations and get feedback from the residuals. If the results are diverging even at small under relaxation factors; it means that there is an inherent problem in the problem setup or some conditions that are applied are incorrect.

Chapter 6

Results and Discussions

The results and discussions sections will shed light upon the results that were obtained from the simulation and will try to derive certain conclusions from the results which will be helpful in further study of gasification and its practical application.

Temperature Gradients Results

The temperature gradient contours are obtained from the Ansys Fluent post processing.

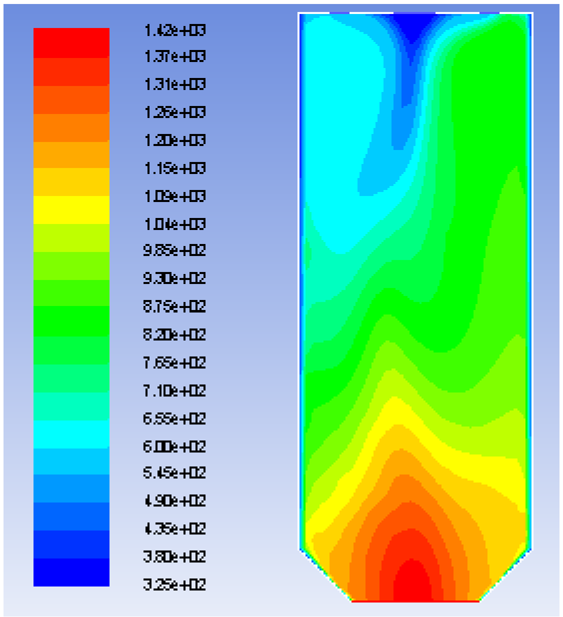


Fig. 11

It can be seen that the coal enters the gasifier at a low temperature (343 K) whereas the air is preheated at 573K. As the reaction takes place the temperature rises down the gasifier. The maximum temperature 1420K is found around the exit which means that the reaction is going on when the mixture leaves the gasifier.There is a requirement of an incomplete reaction which results in the formation of gases that are combustible.

Pressure Contour Results

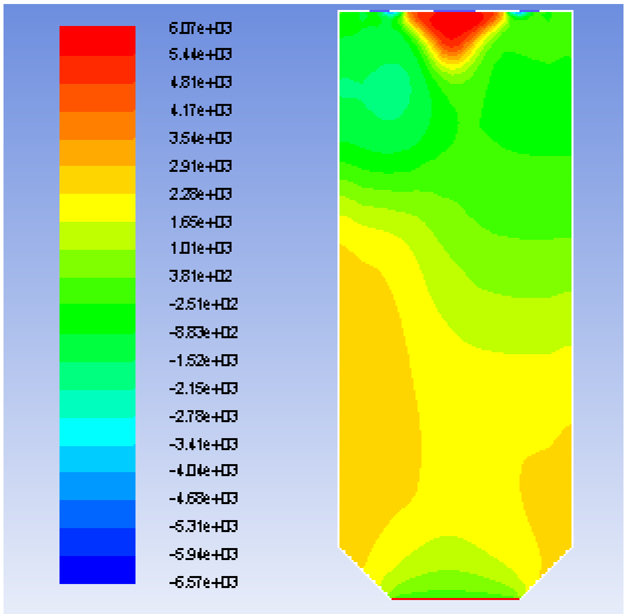


Fig. 12

The pressure contour shows that the maximum pressure is observed at the entrance of the coal slurry and there are low pressure regions around the coal slurry entrance. This is because of low velocity of coal slurry as compared to high velocity of air entering from its two sides. There is again a rise in pressure as the reaction takes place downstream in a confined space from the entrance.

Species Molar Concentration Contours

The discussion about the concentration of different species is given below:

Concentration of O2

The concentration of oxygen is maximum at the top, which is understandable and it gradually decreases downstream. The reason for this decrease is that the oxygen reacts with the coal slurry forming different products. The contour for the molar concentration of O2 is given below in figure 13.

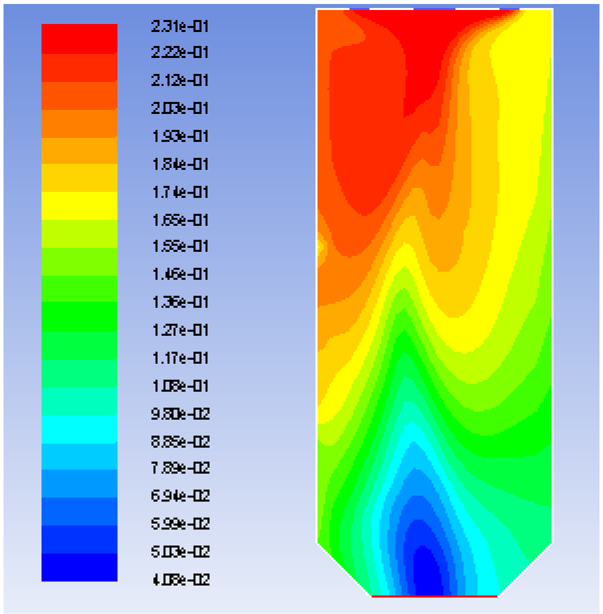


Fig. 13

Concentration of CO

The molar concentration of carbon monoxide is shown in the following figure 14. It can be seen that the concentration of Carbon monoxide is maximum in the middle of the gasifier which signifies the location of reaction 1 i.e. the intermediate stage of the total reaction. It can be seen that a lot of Carbon monoxide is leaving the gasifier.

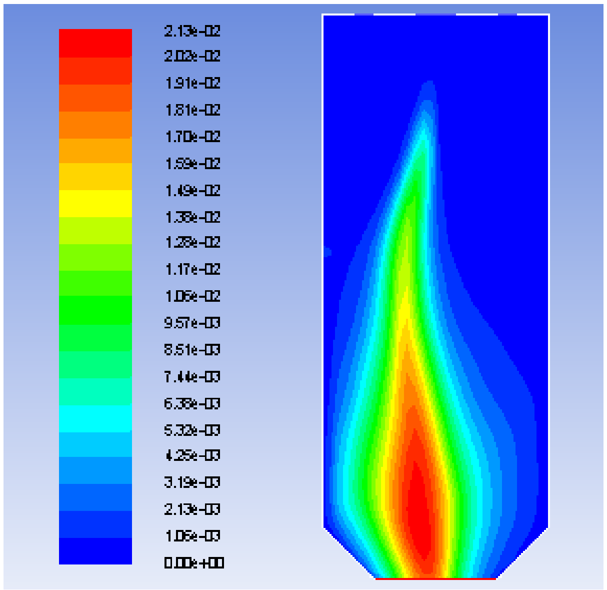


Fig. 14

Concentration of CO2

The molar concentration of CO2 can be seen in the following contour figure. It can be seen that the concentration of CO2 rises downstream as the reaction takes place. CO2 is formed as a product of reaction-1 and reaction-2.

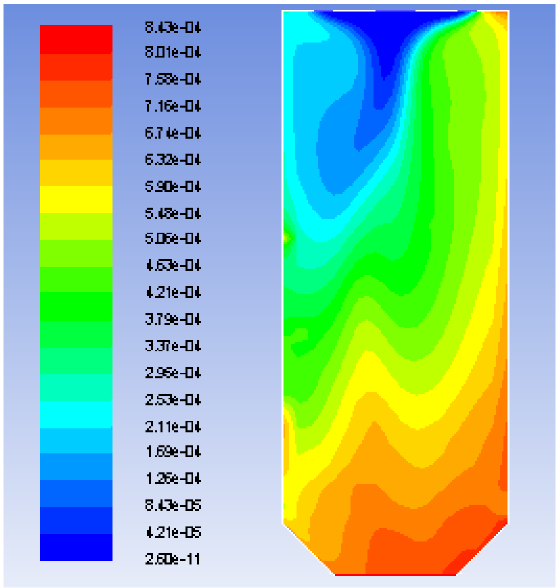


Fig. 15

Concentration of H2O

H2O is formed as a product from reaction-1. It forms a big part of the products that leave the gasifier. The molar concentration of H2O is shown in figure 16 below.

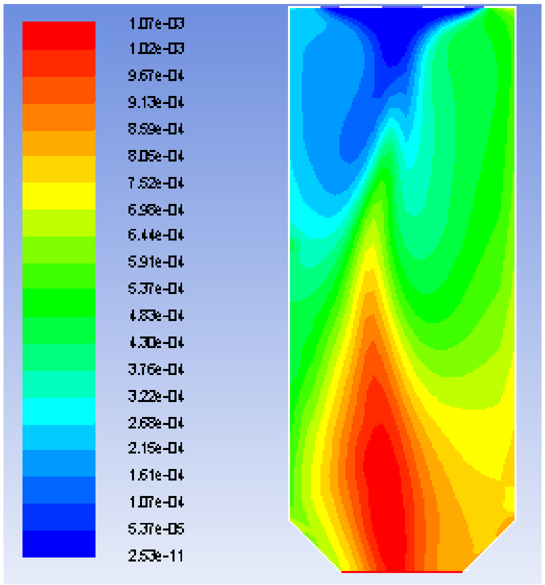


Fig. 16

It can be seen that the concentration contours of H2O and CO are similar because they both are a product of reaction-1.

Rate of Reaction-1

The rate of reaction can also be shown by a contour for turbulent reaction-1 the following contour shows that the reaction starts from the top and is maximum near the top.

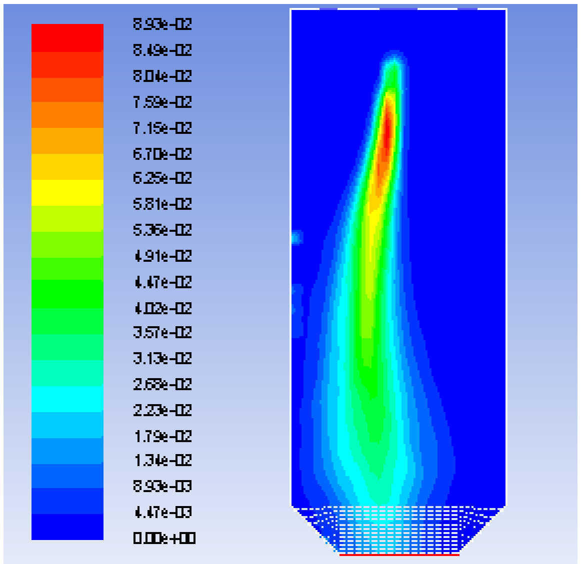


Fig. 17

Rate of Reaction-2

The rate of reaction can also be shown by a contour for turbulent reaction-1 the following contour shows that the reaction is placed below reaction-2

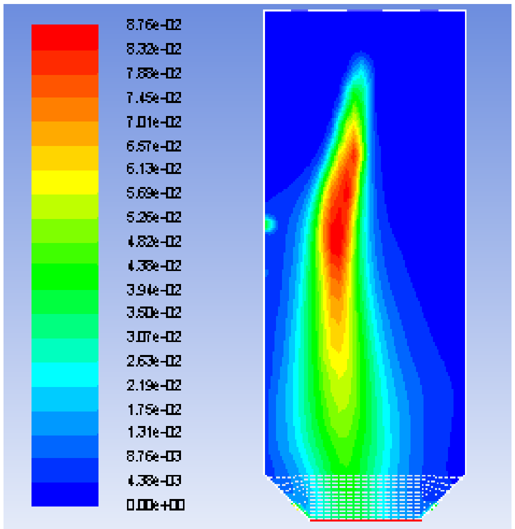


Fig. 18

Chapter 7

Discussion

It is observed that a significant amount of carbon monoxide is being released by the gasifier which can be used for further combustion. According to the charts the mass flow rate of carbon monoxide is 0.467 kg/s. According to the reaction of combustion of carbon monoxide:

$2CO + O_2 \rightarrow 2CO_2$ (Heat of Reaction = 110.53 kJ/mol)

The heat of reaction for each kg of carbon monoxide is 3.948 kJ/ kg

For our given amount of carbon monoxide the energy produced by burning gasified products will be

3.948x 0.467 = 1.844 kJ/s

So heat of 1.844 kW is generated by burning 1.826 kg/s coal.

CO produced:

The amount of carbon monoxide is plotted on different points on the gasifier exit. The carbon monoxide will produced can be used for further burning.

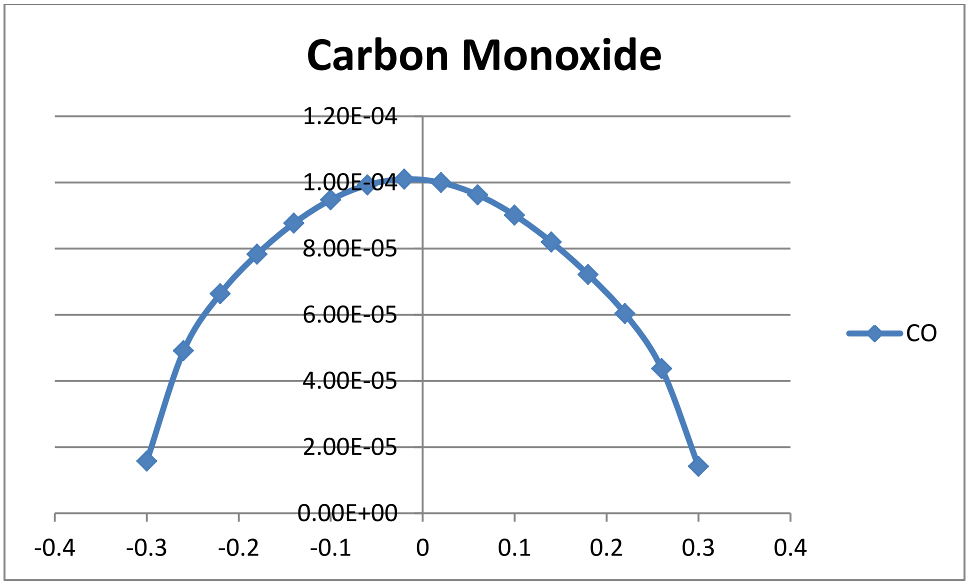


Fig. 19

It can be concluded that the fuel produced from the gasifier does not have sufficient enough calorific value to make the further process of burning feasible.

Chapter 8

Conclusion

The study conducted in this report indicates that the coal present in Thar is of low quality and mostly consists of moisture. If the coal is transported to a far off location for burning the price per unit of energy (Rs/kJ) is high and it becomes unfeasible to mine this coal. However if the coal is burned or gasified at site the transportation cost is saved. If fuel for burning is needed at a present power plant for burning then it is more feasible for the coal to be gasified at site and the product gas to be pumped through a pipeline. A major problem in the gasification is that a lot of energy is wasted to maintain a high temperature in the gasifier with moisture content of almost fifty percent. Most of the energy is lost in the form of latent heatof evaporation due to high moisture content. So it is advisable to use a drying technique to remove as much moisture as possible before starting the gasification process.

As the calorific value of the product gas is not sufficient it is recommended that burning of coal after drying process will be more feasible for power production. It is also recommended that for the power plants to be installed close to the location of coal mines to save on the transportation cost.

Further working can be done in the field of gasification of Thar coal with the deployment of other models as researched before. Experimental study of gasification of Thar coal is also recommended which will help us determine important information and data that can be used to verify our computational findings.

It is imperative that Pakistan makes use of this coal reserve to secure its energy future and economic growth. The oil imports are weighing heavy on the budget and foreign reserves and are a source of increased foreign dependency. The increase in the use of coal will have positive effects on the economy and will help in the eradication of load shedding from the country which is the most popular political slogan in Pakistan.

Utilization of coal through direct burning and through clean coal technologies will help Pakistan in building a green energy culture and will also encourage further research in this field. Through this work it is hoped that new horizons of research will open up that will improve the performance of coal gasification and optimize the process through the use of Thar coal.

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