CFD MODELING OF FLUID CATALYTIC CRACKING RISER REACTOR

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Submitted By

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DECLARATION

I hereby declare that thesis entitled **"CFD Modeling of Fluid Catalytic Cracking Riser Reactor"** is an authentic record of my own work carried out as per the requirements for the award of the degree of **M.Tech. (Chemical Engineering)** at **Thapar University, Patiala**, under the guidance of **Dr. R.K.Gupta**, Associate Professor, **Department of Chemical Engineering**, Thapar University, Patiala during **July 2011 to July 2012**. The matter embodied in this thesis has not been submitted in part or full to any other university or institute for the award of any degree.

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It is certified that the above statement made by the student is correct to the best of my knowledge and belief.

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ABSTRACT

Fluid catalytic cracking (FCC) is a process that converts gas oil to more valuable products in a gas-solid circulating fluidized bed. FCC units are used widely in refineries to produce higher value gasoline from heavy oil. Because of the importance of FCCU in refining, considerable effort has been done for the modeling of this unit. In last five decades, the mathematical modeling of FCC unit have matured in many ways but the modeling continues to evolve to improve the closeness of models predictions to the real process whose hardware is ever changing to meet the needs of petroleum refining. Complexity of the FCC process because of unknown reaction mechanism, complex hydrodynamics, and strong interaction between reactor and regenerator, has made it almost impossible to develop a general model for the integrated process.

Many one and two dimensional, two/three phase models of FCC risers have been developed by the researchers. These models cannot capture the complex hydrodynamics of the riser reactor. In recent years, with the increasing computational capabilities, Computational Fluid Dynamics (CFD) has become a robust modeling tool not only for FCC riser reactor systems, but also for different kind of reacting or non-reacting systems in chemical engineering. CFD can provide us with detailed information on flow processes and heat and mass transfer processes. This is a tremendous advantage over traditional methods of obtaining flow and heat transfer data in FCC riser reactors, which are usually limited to few sampling points and are mostly intrusive.

In the present work a two phase flow FCC riser model incorporating a four lump kinetic scheme is presented. The two phase flow (gas-solid) in the riser is modeled using the Eulerian- Eulerian multiphase flow model. The model simulation studies are presented using two cases: gas-solid flow without reaction, and gas-solid flow with reaction. The results for the two phase flow without reaction show that the gas phase velocity decreases along the riser height as the gas loses momentum. The catalyst velocity increases as the catalyst gains momentum. The temperature of the gas phase increases as it gains heat from the hot catalyst, and the catalyst temperature decreases. The results for gas-solid flow with reaction predict the gas phase velocity increase from 4.7 to 14.7 from riser inlet to outlet due to cracking of heavy gas oil to lighter products. The model predicted gas oil conversion 62%, gasoline yield 39%, light gases yield 20%, and coke yield 3%.

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CHAPTER-1

INTRODUCTION

The fluid catalytic cracking unit (FCCU) plays most important role in the economy of a modern refinery as it is used for value addition to the refinery products. The first FCCU came on stream in 1942 during the World War II to fulfill the demand of aviation gasoline. After that there is tremendous research on the FCCU.

FCCU is the heart of a refinery which converts gas oil to some valuable products in a gas-solid circulating fluidized bed. FCC units are used widely in refineries to produce higher value gasoline from gas oil. A schematic depiction of FCC unit is shown in Figure 1. FCC units mainly consists of two basic units, a reactor in which the hot catalyst is brought in contact with the feed (gas oil), and a regenerator in which the coke deposited on the catalyst is burned off for regenerating the catalyst.

The conversion of heavy petroleum fractions to the products takes place in the riser reactor, which is a long tube of length (30-40m) with a proportionally smaller diameter (0.8-1.2m). Catalyst particle residence time in the FCC reactors is normally a few seconds (less than 5 seconds). The preheated gas oil (feed) having initial boiling point of 340^0C or higher at atmospheric pressure and an average molecular weight ranging from about 200 to 600 or higher enters the riser through feed atomizing nozzles and comes in contact with the hot catalyst coming from the regenerator. The feed droplets are vaporized and cracked as they move upward along with the catalyst. Partially vaporized feed droplets along with solid catalyst particles, hydrocarbon liquid and steam produce a three phase flow, which approximately occupy 2–4m of the riser height depending on initial feed droplet diameter and atomizer characteristic.

After complete vaporization of hydrocarbon feed, two phases solid phase (catalyst), gas phase (hydrocarbon vapor and steam) are left in the riser. Catalytic reactions occur in the vapor phase. The expanding volumes of the vapors that are generated are the main driving force to carry the catalyst up the riser. Catalyst and products are quickly separated in the reactor.

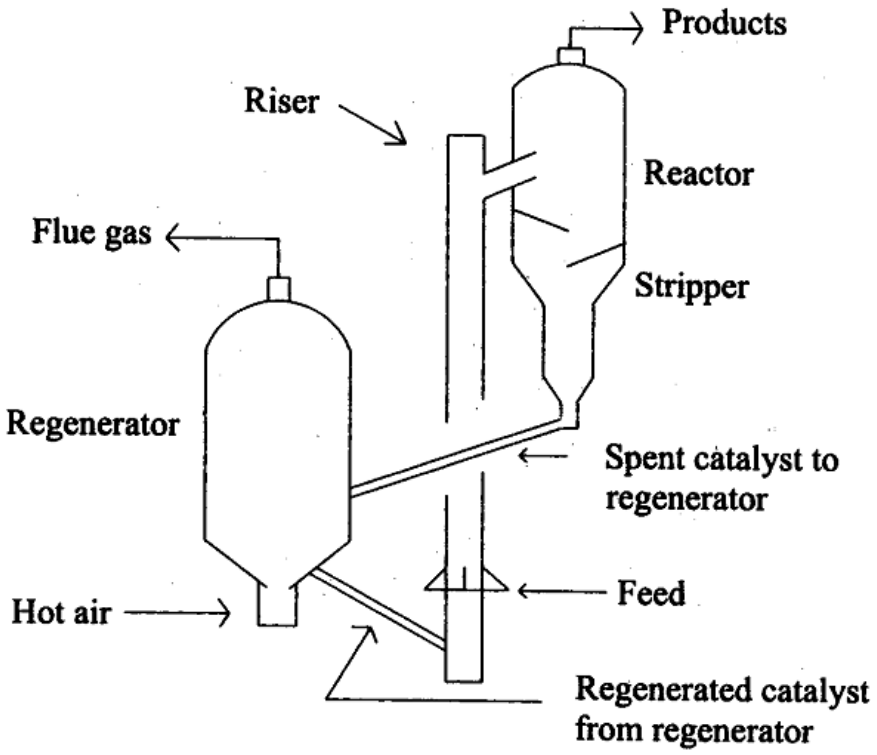


Figure 1: Schematic of FCC unit (Gupta et al., 2005)

After exiting the riser, catalyst entrained by the vapors is separated in the cyclone separators. The cyclones collect and return the catalyst to the stripper. The product vapors exit the cyclones and flow to the main fractionators for recovery. It is important to separate catalyst and vapors as soon as they enter the reactor. Otherwise, the extended contact time of the vapors with the catalyst in the reactor housing will allow for non-selective catalytic re-cracking of some of the desirable products.

In the stripper section, the hydrocarbons adsorbed on the catalyst surface and vapors entrained with the catalyst is separated. Stripping steam is passed at optimum flow rate for the separation of hydrocarbons deposited on the catalyst surface. The hydrocarbons then passed to the main fractionators for their separation into valuable products such as gasoline, light gases and other fractions. Coke, the byproduct of cracking reactions, deposits on the catalyst surface causing the catalyst activity to decrease. The deactivated catalyst is passed to the regenerator.

In the regenerator, coke deposited on the catalyst surface is burned off to regenerate the catalyst. The regenerated catalyst is then again sent to the FCC riser through the stand pipes. The stand pipes provide the pressure to circulate the catalyst around the unit. Thus the catalyst acts as a heat carrier and provides the heat required for the endothermic cracking reactions in the riser reactor and for vaporization of the feed.

CFD is the simulation of fluids engineering systems using modeling (mathematical physical problem formulation) and numerical methods (discretization methods, solvers, numerical parameters, and grid generations, etc.). CFD simulations made possible by the advent of digital computer and advancing with improvements of computer resources.

CFD requires relatively few assumptions and gives a complete description of the flow field of all variables. Quite complex configurations can be treated and the methods are relatively easy to apply. CFD simulations serve as a bridge between theory and reality. Simulations have the advantage that diagnostic probing of a computer simulation does not disturb the flow and normal operation. CFD simulations may allow one to switch on and off various interactions included in the model to understand the relative contributions of each individual process, which is extremely difficult if not impossible to achieve in experiments. These simulations allow detailed analyses at an earlier stage in the design cycle, with less cost, with lower risk and in less time than experimental testing.

But these advantages of CFD are conditional and may be realized only when the fluid dynamics equation are solved accurately, which is extremely difficult for most engineering flows of interest. It must be taken into account that the numerical simulations will always be approximate. There can be various reasons for differences between computed results and experimental results. These include fluid dynamic equations, input data and boundary conditions, numerical methods and convergence, computational constraints, interpretation of results etc. Computational Fluid Dynamics requires broad based expertise in chemical engineering and mathematics and an in-depth understanding of various aspects of the software that is being used to solve the problem. Despite of these limitations, Computational Fluid Dynamics can prove to be of great help to the reactor engineer. The validated computational flow model can be used to evaluate new concepts, designs and configurations. Detailed analyses of the simulations of a flow model will lead to identification of the most promising configurations among the invested configurations, and to

further ideas for evolving new configurations. Though the major process development will no doubt improve of chemical process, there is still a tremendous scope for enhancing performance by harnessing Computational Flow Dynamics.

CFD is emerging as a powerful tool for modeling the FCC riser. In recent decades, with the advancement of computational techniques and computer hardware, CFD is being increasingly used to simulate gas–solid fluidized beds. The hydrodynamics of FCC riser reactor has been studied with different modeling approaches. The accurate analysis of the flow field has not yet been achieved, and most of the times, it is still limited to a two phase flow model. The majority of the research groups have used Eulerian–Eulerian approach, where the dispersed solid particles are treated as an interpenetrating continuum. The kinetic theory of the granular flow is used to simulate gas–solid flow in the riser. Apart from the difficulties in accurate simulations of gas–solid flows, simulation of injected gas oil droplet vaporization and subsequent cracking reactions as well as coke formation reactions is very difficult

In the present work, FCC riser is simulated using Eulerian-Eulerian approach. The vaporization of feed is assumed to be instantaneous. The heat transfer mechanism is described using ranz-marshal correlation. Widely used four lump kinetic scheme is used to predict the product's yields.

CHAPTER 2

LITERATURE REVIEW

Detailed modeling of the riser reactor is a challenging task due to the complex hydrodynamics and involvement of different types of reactions taking place simultaneously. Two main lines of research are found in studies about FCC. One of them takes into account chemical reactions and related phenomena, while not considering some important fluid dynamics aspects. The other set of studies aims to understand the gas–solid hydro-dynamic behavior inside these reactors; without taking into account the reactions involved. The FCC riser is very complex unit to be modeled as it has many aspects to be modeled individually. The various aspects of the FCC riser modeling are reaction kinetics, hydrodynamics, heat and mass transfer and catalyst deactivation. Gupta et al. (2005, 2010) have reviewed the FCC riser modeling efforts of various authors.

2.1 Cracking kinetics

In the FCC riser, thousand of unknown components are present in the feed and many unknown chemical reactions are taking place during the cracking of the petroleum fractions. Due to these facts the modeling of the kinetic mechanism of the fluid catalytic cracking is still a challenge for the researchers. For simplifying the kinetic mechanism of the fluid catalytic cracking, researchers divided the feed and product into components commonly known as lump. For modeling of cracking kinetics, Weekman and Nace (1970) divided the FCC feed stock and products into three lumps: feedstock lump, gasoline lump, and dry gas and coke lump. The light gases and coke is taken as single lump. The main disadvantage of this model is that it only capable of predicting the gasoline yield and does not consider the effect of the coke which gets deposited on the catalyst surface. Coke is mainly the byproduct of the cracking reactions and it provides the heat required for the endothermic reactions. Without considering the effect of the coke, the conversion is not appropriate.

The advancement over the three-lump model is four-lump model. In four-lump model, the lumps are original feedstock, gasoline, light gases and coke. In this model light gases and coke are taken as different lump. Lee et al. (1989) proposed a four lump kinetic model by separating the coke from the three-lump model of Weekman and Nace (1970). The three and four lump schemes are shown in Figure 2 and Figure 3 respectively.

This four lump kinetic scheme was used by several investigators (Gianetto et al., 1994; Ali and Rohani, 1997; Blasetti et al., 1997; Gupta and Subba Rao, 2001; Han and Chung, 2001; Gupta and Subba Rao, 2003; Nayak et al., 2005; Lopez et al., 2011) in their works. There are many studies in which kinetic constants for the four-lump model were estimated (Lee et al., 1989; Farag et al., 1994; Pitault et al., 1995; Blasetti & de Lasa, 1997). The other important kinetic models proposed by various workers: ten lump model (Jacob et al., 1976) and twelve lump model (Oliveira et al., 1987).

But in actual practice, with large number of lumps, the number of kinetic parameters that need to be experimentally obtained increases exponentially. Due to the increase in the kinetic parameters, the system becomes complicated. As a compromise one is constrained to choose the least number of lumps that can provide useful information on yields of marketable products. The four-lump model is generally considered appropriate kinetic model because of its simplicity.

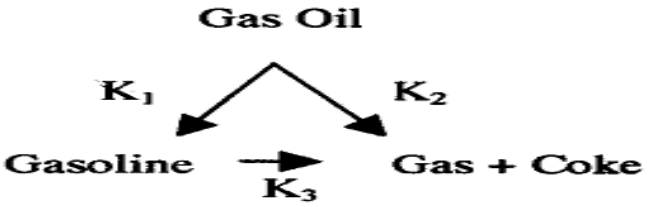


Figure 2: Scheme of three lump (source: Weekman and Nace, 1970)

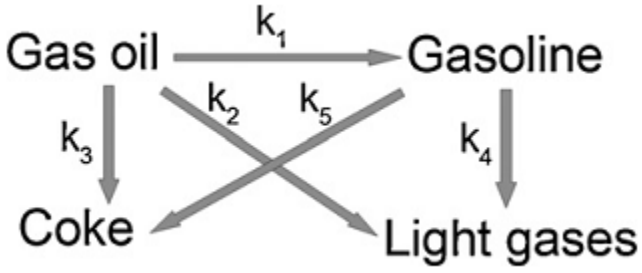


Figure 3: Four lump scheme (Source: Lopes et al., 2011**)**

2.2 Catalyst deactivation

During the cracking reactions, FCC catalyst gets deactivated due to the deposition of coke on the catalyst surface. Most of the popular theories on deactivation are based on the time-on stream concept. Various models for time dependent catalyst decay have been proposed for different lengths of contact time (Weekman, 1968, Nace et al., 1971; Paraskos et al., 1976; Shah et al., 1977). Corella and Menendez (1986) developed a model in which the catalyst surface was assumed to be non-homogeneous with acidic sites of varying strength. There is no specific function that can be used for the deactivation. Different empirical equations have been used by various researchers to fit their experimental data. However, there are two functions that fit the experimental data quite well: power function and exponential function. The exponential function is more widely used.

2.3 Heat and mass transfer

Many riser models assume instantaneous thermal equilibrium between the vapor and solid phases at the riser inlet. The heat transfer between phases has an important role in the catalytic cracking of the hydrocarbons After complete vaporization of feed droplets occurs, a vapor phase and a solid phase exist in the riser. There is considerable temperature difference in these phases near the bottom of the riser. Since, the temperature influences the reaction rates. Prediction of inter-phase heat transfer becomes important.

Considering mass transfer resistance between the phases helps in predicting the concentration of the reacting species at the catalyst surface. Most works have modeled mass transfer using Sherwood's correlation for single particle.

2.4 Hydrodynamics

The another main aspect of the riser modeling is its hydrodynamics. In the hydrodynamics, we mostly study the flow behaviour of feed (liquid droplets/gas) and catalyst. Merry (1971) and Chen and Weinstein (1993) worked on the automization of the feed through nozzles. The feed is sprayed in the riser through nozzles. Yen et al. (1985), and Maoleon and Courefle (1985) worked on the design of the nozzles. They compared single nozzzle and multiple nozzles. The multiple nozzles have smaller size of the droplets. The atomization of feed into fine drops facilitates high

rates of heat transfer between catalyst and feed. This results in a rapid fall in temperature of catalyst in the riser entry zone as it loses heat to hydrocarbon feed. Large drops lead to high catalyst temperature in the riser due to low rates of heat transfer between catalyst and hydrocarbon feed. High catalyst temperature causes high catalyst loading which futher causes slower vaporization rates and low gas velocities. The older nozzle designs with larger droplets causes high catalyst temperature and high catalyst to feed ratio. These facts lead to the secondary cracking reactions. These secondary reactions make the product to crack and decrease the yield which is really undesirable. So, the older nozzle's design which produces larger droplets are surmounted by the multiple nozzle design.

After complete vaporisation the riser has only two phses i.e. vapor phase and solid phase. There is considerable back mixing of the solids due to the slip between the gas and solids. The slip makes difficult in understanding radial profiles of solid velocity difficult. Some of the researchers model the unit by variying the slip velocities. The researchers considered the high slip velocities with core-annulus flow. In this case, flow is divided into two regions-one is turbulent core region in the centre and annulus region near the wall. The researchers concluded that there is high velocity profile in the core and zero velocity profile near the wall i.e. in the annulus region. It is compatible with the experimental data.

The most popular approach in modeling of FCC riser reactor has been the 1-D plug flow model with slip between the phases (Froment and Bischoff, 1990). Although the modeling is simple, these studies obtained good results for the gas oil conversion and product yields at the reactor outlet and some of them could reproduce some axial hydrodynamic aspects. In the two-dimensional models, radial profile is also considered in conjuction with axial profiles. Martin et al. (1992), Fligner et al.(1994), Derouin et al. (1997), and Berry et al. (2004) have all reported two-dimensional models for FCCU risers. They observed that the two-dimensional model provided a better approximation of the results for gas oil conversion and the yields for the species to the industrial data.

2.5 CFD modeling

CFD is emerging as a powerful tool for modeling the FCC riser. In recent decades, with the advancement of computational techniques and computer hardware, CFD is being increasingly used to simulate gas–solid fluidized beds. In the FCC riser, hydrodynamics is complex and there are unknown multiple reactions coupled with mass transfer and heat transfer resistances. The conditions keep changing all along the riser height due to cracking of hydrocarbon feed. Due to these factors, the modeling of FCC riser reactor is very difficult. In recent years, many researchers have modeled the FCC riser reactor using CFD. The hydrodynamics of FCC riser reactor has been studied with different modeling approaches. The accurate analysis of the flow field has not yet been achieved, and most of the times, it is still limited to a two phase flow model. Apart from the difficulties in accurate simulations of gas–solid flows, simulation of injected gas oil droplet vaporization and subsequent cracking reactions as well as coke formation reactions is very difficult (Behjat et al., 2010).

There are two approaches for the numerical calculation of multiphase flows: the Euler-Lagrangian approach and the Euler -Euler approach. The majority of the research groups have used Eulerian–Eulerian approach, where the dispersed solid particles are treated as an interpenetrating continuum. The kinetic theory of the granular flow is used to simulate gas–solid flow in the riser.

Euler-Langrangian approach: In this approach, the fluid phase is treated as a continuum by solving the time-averaged Navier-Stokes equations, while the dispersed phase is solved by tracking a large number of particles, bubbles, or droplets through the calculated flow field by taking into account the effects of particle collisions and forces acting on the particle by the gas. In this approach, equations are derived by considering a control volume (material volume) such that the velocity of the control volume surface always equals the local fluid velocity. The dispersed phase can exchange momentum, mass, and energy with the fluid phase. A fundamental assumption made in this model is that the dispersed second phase occupies a low volume fraction, even though high mass loading ($m_{particles} \geq m_{fluid}$) is acceptable. The particle or droplet trajectories are computed individually at specified intervals during the fluid phase calculation. This makes the model appropriate for the modeling of spray dryers, coal and liquid fuel combustion, and some particle-laden flows, but inappropriate for the modeling of liquid-liquid

mixtures, fluidized beds, or any application where the volume fraction of the second phase is not negligible.

Euler- Euler approach: In this approach, the different phases are treated mathematically as inter-penetrating continua. Since the volume of a phase cannot be occupied by the other phases, the concept of phasic volume fraction is introduced. In this approach, an arbitrary control volume in a stationary reference frame is used to derive the basic governing equations. These volume fractions are assumed to be continuous functions of space and time and their sum is equal to one. Conservation equations for each phase are derived to obtain a set of equations, which have similar structure for all phases. These equations are closed by providing constitutive relations that are obtained from empirical information, or, in the case of granular flows, by application of kinetic theory. In FLUENT, three different Euler-Euler multiphase models are available: the volume of fluid (VOF) model, the mixture model, and the Eulerian model.

*VOF model***:** This model is a surface tracking technique applied to a fixed Eulerian mesh. It is designed for two or more immiscible fluids where the position of the interface between the fluids is of interest. In the VOF model, a single set of momentum equations is shared by the fluids, and the volume fraction of each of the fluids in each computational cell is tracked throughout the domain. Applications of the VOF model include stratified flows, free-surface flows, filling, sloshing, the motion of large bubbles in a liquid, the motion of liquid after a dam break, the prediction of jet breakup (surface tension), and the steady or transient tracking of any liquid-gas interface.

Mixture model: This model is designed for two or more phases (fluid or particulate). As in the Eulerian model, the phases are treated as interpenetrating continua. The mixture model solves for the mixture momentum equation and prescribes relative velocities to describe the dispersed phases. Applications of the mixture model include particle-laden flows with low loading, bubbly flows, sedimentation, and cyclone separators. The mixture model can also be used without relative velocities for the dispersed phases to model homogeneous multiphase flow.

Eulerian model: The model is the most complex of the multiphase models in FLUENT. It solves a set of n momentum and continuity equations for each phase. Coupling is achieved through the pressure and interphase exchange coefficients. The manner in which this coupling is handled

depends upon the type of phases involved; granular (fluid-solid) flows are handled differently than non-granular (fluid-fluid) flows. For granular flows, the properties are obtained from application of kinetic theory. Momentum exchange between the phases is also dependent upon the type of mixture being modeled. Applications of the Eulerian multiphase model include bubble columns, risers, particle suspension, and fluidized beds.

Eulerian-Eulerian models consider both gas and solid phases as continuous and fully interpenetrating. The equations employed are a generalization of the Navier–Stokes equations for interacting continua. Owing to the Eulerian representation of the particle phases, Eulerian-Eulerian models require additional closure laws to describe the rheology of particles. In most recent continuum models constitutive equations according to the kinetic theory of granular flow are incorporated.

For FCC riser modeling, most works used Eulerian–Eulerian approach where the dispersed solid particles are treated as interpenetrating continuum (Theologos and Markatos, 1993; Benyahia et al., 2003; Zimmermann and Taghipour, 2005; Lan et al. 2009). Few works have used Eulerian–Lagrangian approach (Nayak et al. 2005; Wu et al., 2010). In this approach, the motion of solid catalyst particles is modeled in the Lagrangian framework and the motion of continuous phase is modeled in the Eulerian framework. This approach offers a more natural way to simulate complex particle level processes like cracking reactions. Also, heat and mass transfer and chemical reactions occurring at the individual particle scale can be conveniently accounted using this approach. The approach however requires significantly more computational resources and therefore rarely used for dense gas–solid risers.

Many efforts have been made in feed injection design to control the flow of the catalyst and hydrocarbons in plug flow conditions in order to minimize the undesirable temperature gradients, which may result in undesirable cracking reactions. Most of the works on the FCC riser reactor have focused on either reactor hydrodynamics or catalytic cracking kinetics. Many theoretical and experimental studies are carried out to better understand the complex hydrodynamics of gas–solid turbulent flow in the reactor (Gao et al., 1999; Huilin et al., 2003; Goldschmidt et al.,2004; Jiradilok et al., 2006; Wang et al., 2008; Wang and Liu, 2010;). Most of the experiments and simulations were carried out in cold flow modes, excluding the influence of heat transfer and cracking reactions. Chang et al. (2001) have proposed a three phase reacting flow CFD model to

study the effects of droplet injection parameters on the FCC riser performance. They have reported the optimum operating conditions for the spray injection.

Gao et al. (1999) developed a model that predicted three-dimensional, two-phase flow inside the riser-type reactor. The authors used a thirteen lump kinetic scheme and demonstrated that excessive cracking occurred beyond the 10 m riser height, and resulted in the increase of by-products yield at the expense of desirable products. Authors further extended this model to three-phase flow model (Gao et al., 2001) by incorporating the effect of feed vaporization.

Benyahia et al. (2001) proposed the physical process as a gas/solid multiphase flow with reaction. A transient Eulerian approach plus a simple 3-lumps reaction kinetic scheme (Nace et al., 1971) describe the multiphase flow model. The gas density was assumed to follow an ideal gas law, and can, thus, change with the number of moles in the system. Conservation of mass, momentum, and species (heavy oil, gasoline and gas+coke) were solved. The gas/solid hydrodynamics and the yields of the reacting species were predicted in the 2-D Riser section of the FCC unit. The results showed a dramatic effect of the change in the number of moles of the chemical species on the hydrodynamics. The increase in the number of moles due to the cracking reactions resulted in a significant increase in the gas flow rate, which changed significantly the flow regime. The reaction yields compared reasonably well with the design data for this specific unit.

Huilin et al. (2005) used a cluster based approach and predicted the hydrodynamics of cluster flow in circulating fluidized beds. Authors showed a considerable improvement in the model predictions using cluster based approach as compared to the model based on original kinetic theory of granular flow.

Jiradilok et al. (2006) proposed the turbulent fluidization of FCC particles in a riser. The turbulent fluidization regime is characterized by the co-existence of a dense, bottom region and a dilute, top bed. A kinetic theory based CFD code with a drag corrected for clusters captured the basic features of this flow regime: the dilute and dense regions, high dispersion coefficients. A turbulent fluidized bed is characterized by two different co-existing regions: a bottom dense, bubbling region and a dilute, dispersed flow region. The solids volume fractions in these two regions can be estimated using the drift flux method. The hydrodynamic model for the

multiphase flow is based on the generalization of Navier–Stokes equations. It uses the Eulerian–Eulerian approach.

Novia et al. (2007) work on the one of the most uncertain aspects of a fluid catalytic cracking (FCC) unit, which is the description of fluid-solid mixing at the riser entrance. Most of the existing models assume an instant mixing of solids and gaseous reactants. However, a finite mixing length at the bottom of the riser may have a pronounced effect on the FCC operation, particularly, when very short residence times are allowed in the current commercial FCC risers. A good solid-fluid mixing is essential to ensure a complete feed vaporization which is important for several reasons including assuring a thorough catalyst to oil contact and minimizing coke deposition. The author used the Eulerian-Eulerian multiphase flow and the 3-lump kinetic models to simulate the hydrodynamics and cracking reactions occurring in the FCC riser reactors. The model demonstrated the capability of commercial CFD code FLUENT 6.2 to describe the flow field in the riser reactor. The model also takes into account the temperature, the heat of reactions and gasoline distribution along the riser height.

Shuyan (2008) proposed a mathematical model for predicting gas and gasoline distributions in the cluster by coupling a hydrodynamics model with four-lump catalyst cracking reactions. The author investigated the effects of the cluster porosity, inlet gas velocity and temperature, and coke deposition on cracking reactions of the cluster. The reaction rates from vacuum gas oil (VGO) to gasoline, gas and coke of individual particle in the cluster are higher than those of the isolated particle, but it reverses for the reaction rates from gasoline to gas and coke. The produced mass fluxes of gas and gasoline increase with the operating temperature and molar concentration of VGO, and decrease due to the formation of coke. Flow and cracking reactions have been predicted by using a three-dimensional computational fluid dynamics (CFD) models for FCC riser with Eulerian approach and reactions with lumping models.

Lu et al. (2008) presented a gas-solid multi-fluid model with two granular temperatures of the dispersed particles and the clusters in risers, to predict the hydrodynamics of dispersed particles and clusters flow in CFBs. In addition to the basic governing equations developed from the universal laws, it is necessary to develop relevant constitutive equations and equations of state for the fluids under consideration to close the system of equations. Several closure models have been proposed to define the appropriate constitutive equations for binary or multi-phase flows

based on the kinetic theory of granular flow. The constitutive equations are needed to close the solid phase momentum

Behjat et al. (2010) proposed a 3-D FCC riser reactor model, which takes into account the hydrodynamics, heat transfer and evaporation of the liquid gas oil injected into the gas–solid fluidized bed. The source terms appearing in the mass, momentum and energy equations represent the interactions between the droplets and the gas and solid phases. The CFD simulation results indicated that residence times for gas oil droplet were affected by the type of the drag model. The drag force was the dominant force in the feed droplet hydrodynamic. The rapid evaporation of the droplets has a significant effect on the gas–solid flow mixing, the gas–solid phase flow field and the temperature near the atomizer region. The CFD simulation showed that droplet evaporation led to an excessive vapor production that was distributed into the surrounding gas stream, causing higher local velocities of the gas and solid particles and lower solid concentrations as well as solid particle temperature reduction. These variations, in turn could affect the process efficiency.

Lopes et al. (2011) developed a model of three-dimensional and two-phase flow model to predict the dynamic behavior of a fluid catalytic cracking (FCC) industrial reactor. The study took into account heat transfer and chemical reactions. A four-lump model was proposed to represent the catalytic cracking reactions in which the heavy oil (gas oil) is converted into gasoline and light hydrocarbon gases. Gas acceleration inside the reactor due to molar expansion and a model to describe undesirable catalyst deactivation by coke deposition on its surface were also considered. An Eulerian description of the phases was used to represent the two-phase flow.

CHAPTER-3

FCC RISER MODEL

Modeling of the riser reactor of an FCC unit is quite complex because of the presence of all three phases inside the reactor, involvement of physical and chemical rate steps, and its strong interaction with the regenerator. Nevertheless, considerable efforts are being made by various workers in all the aspects of riser modeling.

With the development of high performance computers and advances in numerical techniques and algorithms, computational fluid dynamics (CFD) tools are increasingly gaining popularity. Some information such as turbulence parameters, which cannot be obtained or are hard to obtain in laboratory conditions, are easily estimated using CFD tools. In addition, CFD models provide a more detailed data profile as a function of space and time without interfering or disturbing the flow by internal probes. Although modeling tools help explain the fluid behavior more accurately, experimental studies are required to evaluate any multiphase CFD model.

In this chapter the numerical model of the FCC riser is presented. The model incorporates a four lump kinetic model, and two-phase flow

Riser hydrodynamics

The two-phase flow model uses Eulerian description of both phases, so the gases and the dispersed solid particles are treated as interpenetrating continuum. The governing conservation equations are the following:

Continuity equations

The gas and solid phase continuity equations are given respectively by:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g\right) + \nabla.\left(\varepsilon_g \rho_g u_g\right) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s\right) + \nabla.\left(\varepsilon_s \rho_s u_s\right) = 0 \quad (2)$$

where ε stands for the volume fraction, for the density and u for the velocity of each phase. The subscripts g and s indicate the gas and particulate phases, respectively. No mass transfer is considered to occur between the phases.

Momentum equations

The gas and solid phase momentum equation may be expressed as:

$$\frac{\partial}{\partial t}(\varepsilon_g \rho_g u_g) + \nabla.(\varepsilon_g \rho_g u_g u_g) = \nabla.\left[\varepsilon_g \mu_g \left(\nabla \mathrm{u_g} + (\nabla \mathrm{u_g})^{\mathrm{T}}\right)\right] + \varepsilon_g \rho_g g - \varepsilon_g \nabla p + \beta(u_s - u_g) \quad (3)$$

$$\frac{\partial}{\partial t}(\varepsilon_s \rho_s u_s) + \nabla.(\varepsilon_s \rho_s u_s u_s) = \nabla.[\varepsilon_s \mu_s (\nabla \mathrm{u_s} + (\nabla \mathrm{u_s})^{\mathrm{T}})] + \varepsilon_s \rho_s g - \varepsilon_s \mathrm{G} \nabla \varepsilon_s + \beta(u_g - u_s) \quad (4)$$

where μ is the viscosity, g the acceleration of gravity, p the pressure, G the modulus of elasticity and β is the interphase momentum transfer.

For dense regions (ε_s> 0.2), β is given by:

$$\beta = 150 \frac{\varepsilon_s^2 \mu_g}{\epsilon_g d_s^2} + \frac{7}{4} \frac{|u_s - u_g| \varepsilon_s \rho_g}{d_s} \quad (5)$$

and for dilute regions ($\varepsilon_s < 0.2$), it is given by:

$$\beta = \frac{3}{4} C_d \frac{|u_s - u_g| \varepsilon_s \rho_g}{d_s} \quad (6)$$

where d_s is the particle diameter and C_d is the drag coefficient. In the present work, Syamlal-O'Brien drag model is used.

Turbulence equations:

The gas-phase effective viscosity was predicted as a sum of the molecular viscosity and an eddy contribution:

$$\mu_g = \mu_{lam,g} + \mu_{turb,g} \quad (7)$$

In the present work the turbulent viscosity was modeled using the k-epsilon model. The simplest "complete models" of turbulence are the two-equation models in which the solution of two separate transport equations allows the turbulent velocity and length scales to be independently

determined. Robustness, economy, and reasonable accuracy for a wide range of turbulent flows explain its popularity in industrial flow and heat transfer simulations. It is a semi-empirical model, and the derivation of the model equations relies on phenomenological considerations and empiricism. In this model the eddy viscosity is given as the ratio between the turbulent kinetic energy (k) and its dissipation rate (ϵ):

$$\mu_{turb,g} = C_\mu \rho_g \frac{k^2}{\epsilon} \tag{8}$$

where C_μ is a constant. The values of k and ϵ come directly from the differential transport equations for the kinetic energy and turbulence dissipation rate as follows:

$$\frac{\partial}{\partial t}\left(\rho_g k\right) + \nabla.\left(\rho_g u_g k\right) = \nabla.\left[\left(\mu_{lam,g} + \frac{\mu_{turb,g}}{\sigma_k}\right)\nabla k\right] + P^k - \rho_g \epsilon \tag{9}$$

$$\frac{\partial}{\partial t}\left(\rho_g \epsilon\right) + \nabla.\left(\rho_g u_g \epsilon\right) = \nabla.\left[\left(\mu_{lam,g} + \frac{\mu_{turb,g}}{\sigma_\epsilon}\right)\nabla \epsilon\right] + \frac{\epsilon}{k}\left(C_{\epsilon,1} P^k - C_{\epsilon,2}\rho_g \epsilon\right) \tag{10}$$

Where $\sigma_k, \sigma_\epsilon, C_{\epsilon,1}, C_{\epsilon,2}$ are constants and P^k is the turbulence production, which is modeled using

$$P^k = \mu_{turb,g} \nabla u_g.\left(\nabla \mathrm{u_g} + \left(\nabla \mathrm{u_g}\right)^{\mathrm{T}}\right) \tag{11}$$

Heat transfer model:

The heat transfer between phases has an important role in the catalytic cracking of the hydrocarbons, since the hot regenerated catalyst in contact with the gas oil feed should provide enough heat for liquid vaporization and endothermic cracking reactions. The gas and solid energy equations are expressed respectively as:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g H_g\right) + \nabla.\left(\varepsilon_g \rho_g u_g H_g\right) = \nabla.\left(\varepsilon_g \lambda_g \nabla T_g\right) + \gamma\left(T_s - T_g\right) + \varepsilon_g \rho_g \sum_r \Delta H_r \frac{\partial C_r}{\partial t} \tag{12}$$

$$\frac{\partial}{\partial t}\left(\varepsilon_s \rho_s H_s\right) + \nabla.\left(\varepsilon_s \rho_s u_s H_s\right) = \nabla.\left(\varepsilon_s \lambda_s \nabla T_s\right) + \gamma\left(T_g - T_s\right) \tag{13}$$

γ is the interphase heat transfer coefficient, which is modeled using the following correlation:

$$\gamma = \frac{Nu\lambda}{d_s} \tag{14}$$

where $d_s$is the mean diameter of the dispersed phase and Nu is the Nusselt number. For a particle moving in an incompressible Newtonian fluid, the Nusselt number is a function of the Reynolds and Prandtl numbers of the particle. The Nusselt number used in this work is estimated by the Ranz–Marshall correlation for single particle:

$$Nu = 2 + 0.6Re^{0.5}Pr^{0.3} \tag{15}$$

Catalytic cracking kinetic model:

The variation in chemical species in the gas phase is modeled as follows:

$$\frac{\partial}{\partial t}\left(\varepsilon_g \rho_g C_{g,i}\right) + \nabla.\left(\varepsilon_g \rho_g u_g C_{g,i}\right) = \nabla.\left(\varepsilon_g \Gamma_i \nabla C_{g,i}\right) + \hat{R}_i \tag{16}$$

where $C_{g,i}$ is the concentration of specie $\hat{R}_i$ in the gas phase, Γ is diffusivity in the phase and $R_i$the consumption/formation of this specie due to the cracking reactions.

In the present work, a four lump kinetic scheme (Figure 4) is used due to its simplicity. The general rate equation for reaction r is given by:

$$R_{i,r} = k_r C_i^n \tag{17}$$

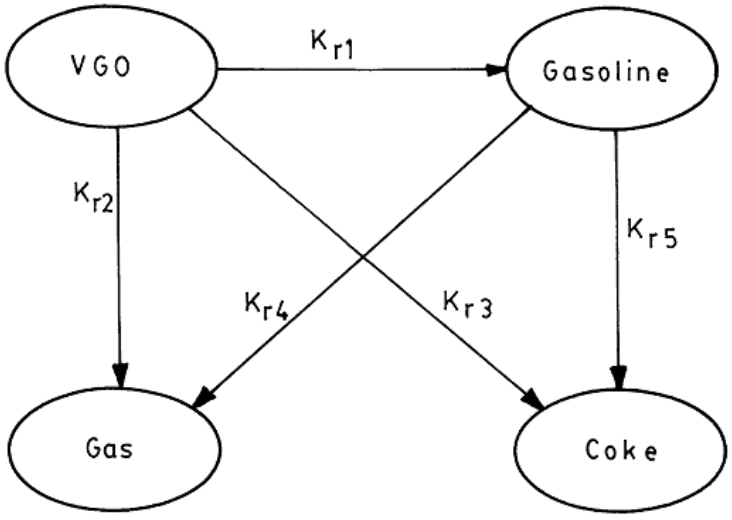


Figure 4: Reaction scheme for four-lump model

The dependence of kinetic constants on temperature is given by Arrhenius equation according to

$$k_r = k_r^0 \, exp\left(\frac{-E}{RT}\right) \tag{18}$$

The values of pre exponential factor and activation energy used in the model are reported in Table 1. The stoichiometric coefficients are given in Table 2.

Table 1 Pre exponential factor and activation energy of four lump model

Reaction	Pre-exponential factor (m^3/ m_{cat}^3.s)	Activation energy E, (kJ/kmol)
Gasoil (VGO) to Gasoline	0.06	68316
Gasoil (VGO) to Light Gases	0.04	89303
Gasoil (VGO) to Coke	0.0076	64638
Gasoline to Light Gases	0.0042	52768
Gasoline to Coke	0	115566

Table 2 Stoichiometric coefficients

Reaction	Stoichiometric coefficients
Gasoil (VGO) to Gasoline	400/100
Gasoil (VGO) to Light Gases	400/50
Gasoil (VGO) to Coke	400/400
Gasoline to Light Gases	100/50
Gasoline to Coke	100/400

Geometry creating and meshing

A cylindrical having diameter 0.8m and height 33m was created for FCC riser and meshing. Total 143226 control elemental volume is formed. Figure 5 gives close look of meshed volume.

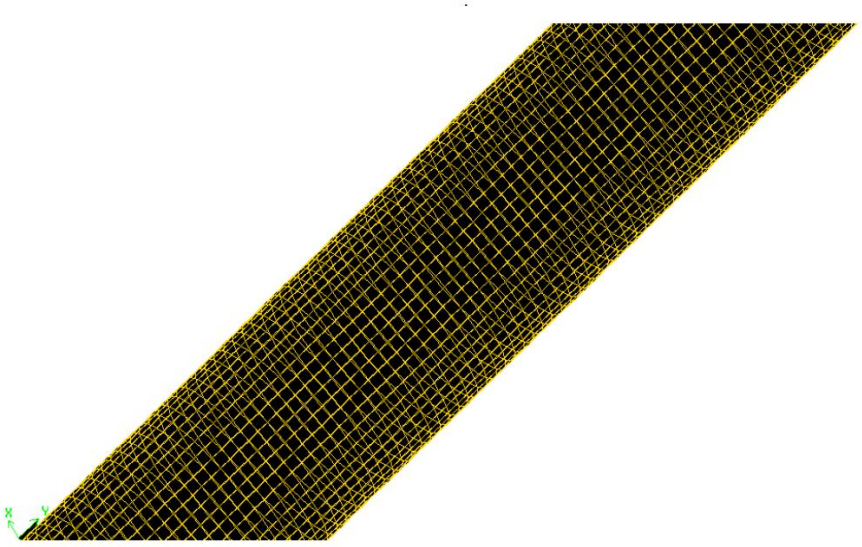


Figure 5: View of riser after meshing

Each element has a value of skewness between 0 and 1, where 0 represents an ideal element. The histogram in Figure 6 is divided into 10 bars; each bar represents a 0.1 increment in the skewness value. For a good mesh, the bars on the left of the histogram will be large and those on the right will be small. The following Figure shows 143226 elements are active and skewness of all elements mostly lies below 0.4. Worst quality element shown in Figure 7 having skewness is 0.427217. Quality ranges are: 0 - 0.1= 64.81%; 0.1 - 0.2=19.44%; 0.2 - 0.3=5.97%; 0.3- 0.4=9.16%

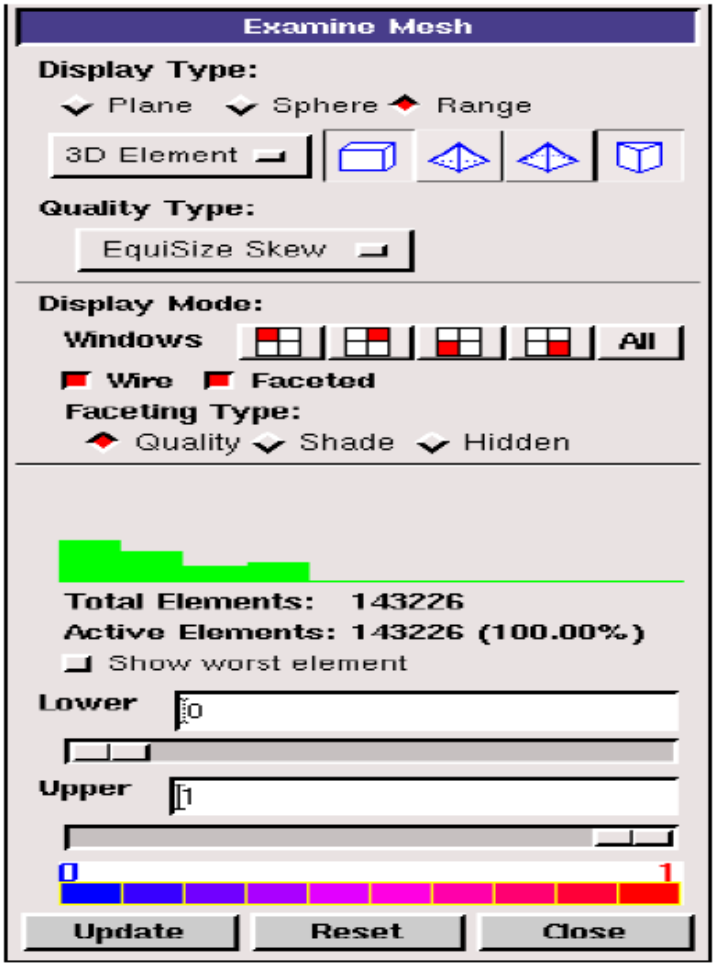


Figure 6: Mesh examine panel

Figure 7: Shape of worst element

Set boundary types

Type of boundary conditions were specified in GAMBIT. Geometry after mesh generation, quality check and specified boundary type shown in Figure 8.

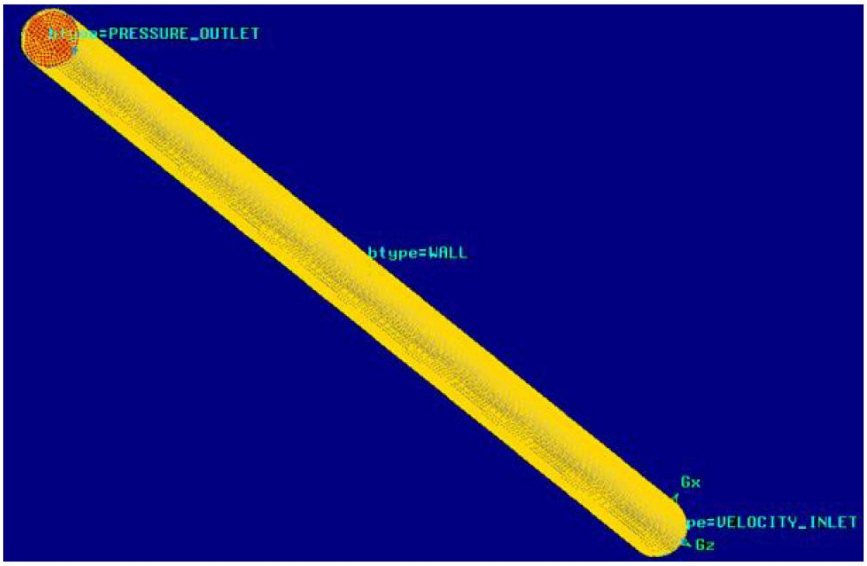


Figure 8: Inflow and Outflow boundaries of FCC riser

Saved the meshed file by option of export mesh. It creates the .msh file in working directory.

Solving

Read the grid .msh file and performed grid check. The minimum volume reported is a positive number. Grid diagram displayed as Figure 9.

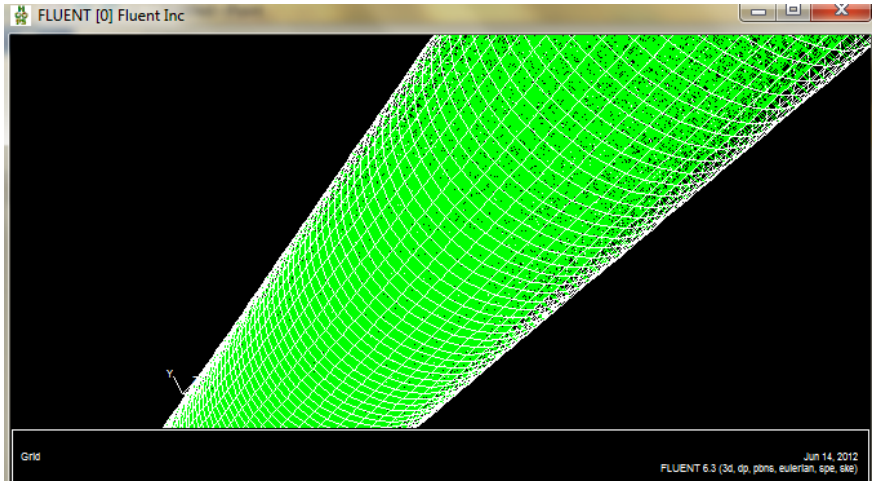


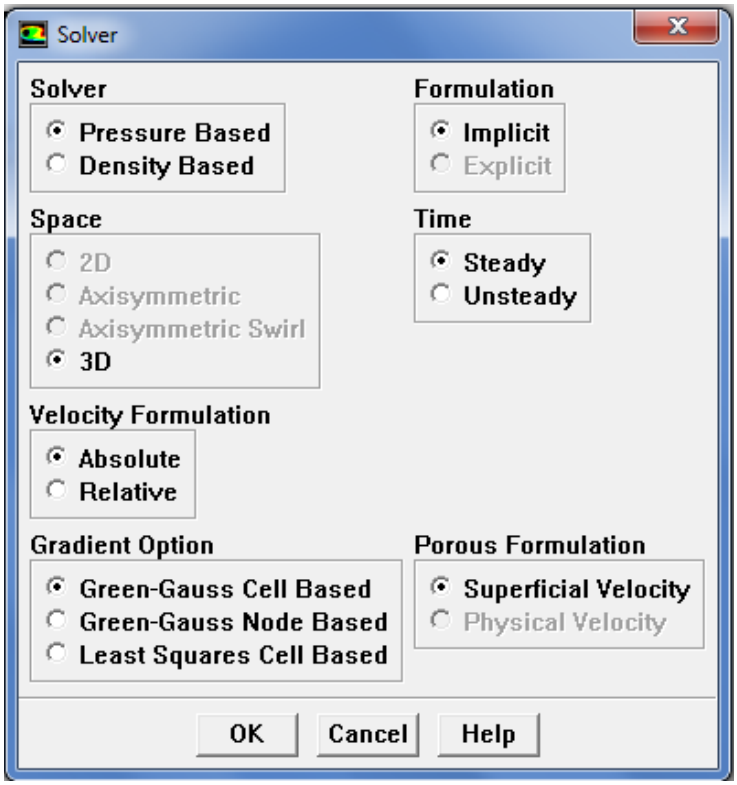
Figure 9: Grid Diagram

```
Grid Check

 Domain Extents:
   x-coordinate: min (m) = -8.000000e-001, max (m) = 8.000000e-001
   y-coordinate: min (m) = -7.984634e-001, max (m) = 7.984634e-001
   z-coordinate: min (m) = 0.000000e+000, max (m) = 3.300000e+001
 Volume statistics:
   minimum volume (m3): 4.489888e-004
   maximum volume (m3): 1.806547e-003
     total volume (m3): 6.617593e+001
 Face area statistics:
   minimum face area (m2): 4.469082e-003
   maximum face area (m2): 1.734764e-002
 Checking number of nodes per cell.
 Checking number of faces per cell.
 Checking thread pointers.
 Checking number of cells per face.
 Checking face cells.
 Checking bridge faces.
 Checking right-handed cells.
 Checking face handedness.
 Checking face node order.
 Checking element type consistency.
 Checking boundary types:
 Checking face pairs.
 Checking periodic boundaries.
 Checking node count.
 Checking nosolve cell count.
 Checking nosolve face count.
 Checking face children.
 Checking cell children.
 Checking storage.
Done.
```

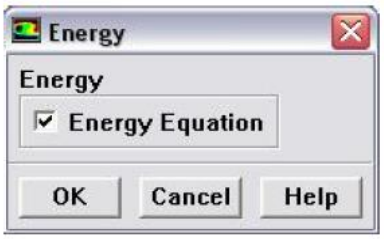
Models

Models specified as pressure based, 3D, velocity formulation as absolute, gradient option as Green-Gauss cell based and porous formulation as superficial velocity.

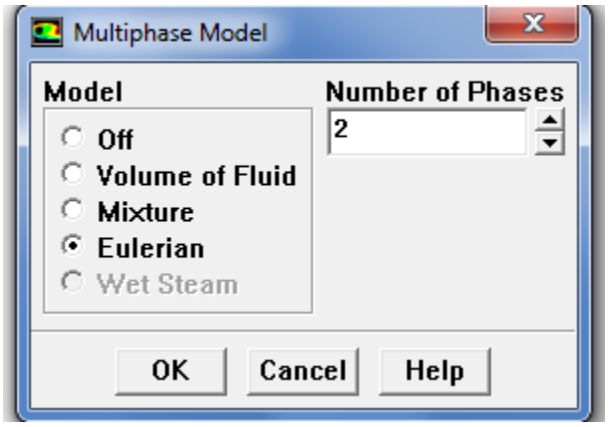


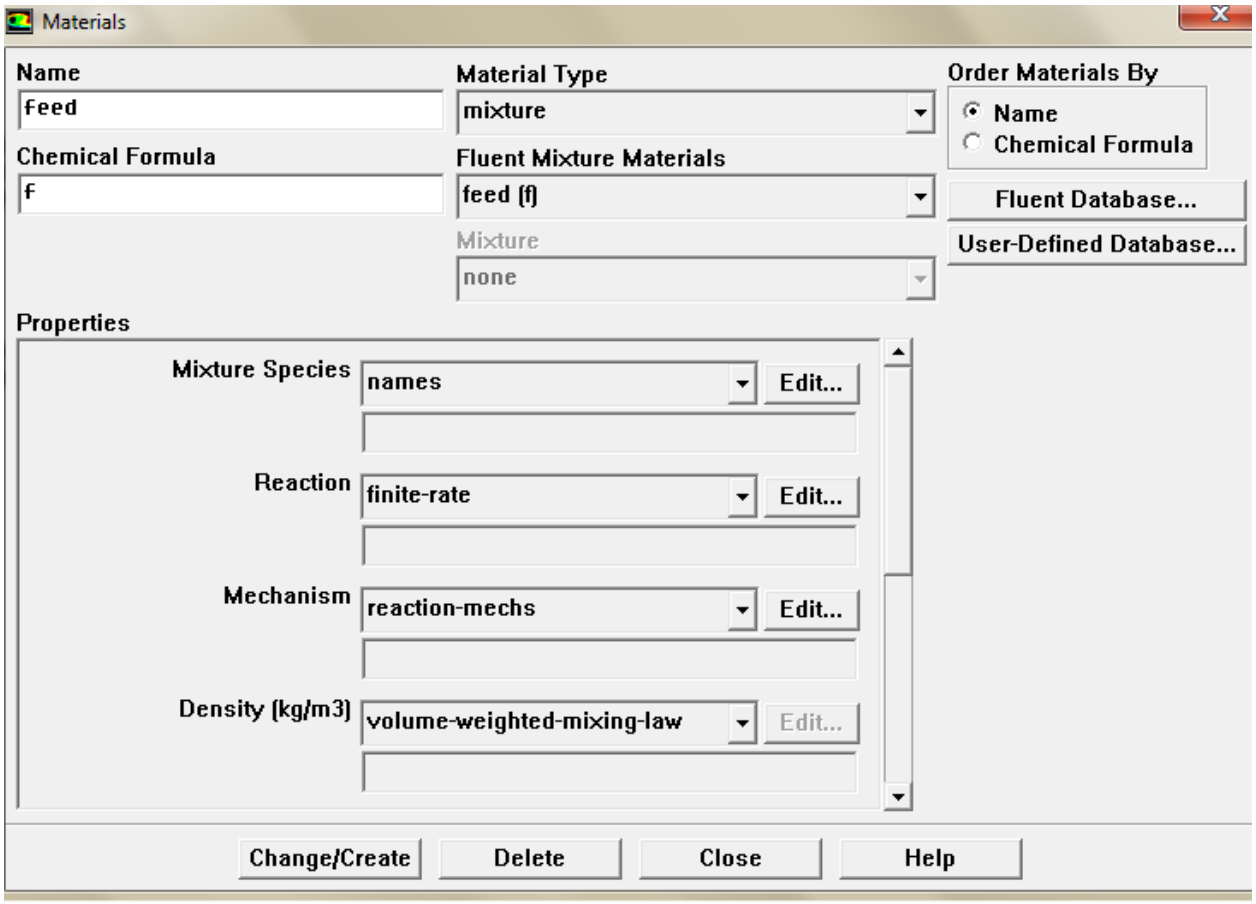
In general, there are two approaches to solving the governing conservation equations: pressure based and density-based solution methods. In pressure-based methods, pressure and velocity are calculated separately in an iterative manner from the continuity and momentum balance equations. However, in density-based methods, all model equations are solved simultaneously and the corrected values of all dependent variables for the next time step are obtained directly; no iterations are needed to satisfy both pressure and momentum. The species model is used for the description of turbulent or laminar conditions.

Enabled energy equation:



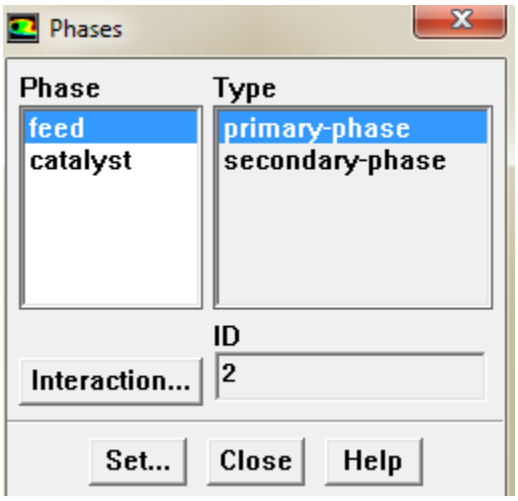
Multiphase model:





Phases

The primary phase is feed vapor, secondary phase is catalyst.



The plant data reported in Table 3 is used for the simulation. The gas oil feed is assumed to be vaporizing instantaneously after gaining sensible heat from the catalyst. Thus, the temperature of vaporized feed at the inlet is taken as 700 K and temperature of the catalyst is taken as 860 K. The gas phase velocity magnitude 4.74m/s and catalyst phase velocity is 0.295m/s.

Table 3 Plant Data (Ali and Rohani, 1997)

Parameter	Value
Feed flow rate	20 kg/s
Catalyst flow rate	144 kg/s
Riser Diameter	0.8 m
Riser Pressure	2.9 atm
Riser height	33 m

CHAPTER -4

RESULTS AND DISCUSSION

The results are organized in two cases. In case 1, the gas-solid flow simulations without reaction are presented. In case 2, the results of gas-solid flow simulations with cracking reactions are presented. For both the cases the gas-oil feed is assumed to be instantaneously converting into vapor after contacting with the hot catalyst coming from the regenerator.

Case 1

The feed vapor drags catalyst particles up the riser and thus loses momentum. There is decrease in the velocity of the gas phase (Figures 10 & 11) and increase in the velocity of the catalyst phase (Figures 12 & 13). The velocity of feed falls initially and then becomes constant. Contour of velocity magnitude (Figure 11) shows maximum velocity at the centre. Also, the velocity is maximum at the inlet and minimum at outlet. The feed is gas-oil vapor which remains unchanged in the riser.

The heat is transferred from catalyst phase to gas phase. The temperature of gas phase (Figures 14 & 15) increases due to heat gain, and catalyst phase (Figures 16 & 17) temperature decreases due to heat loss. Eventually, both phases attain thermal equilibrium.

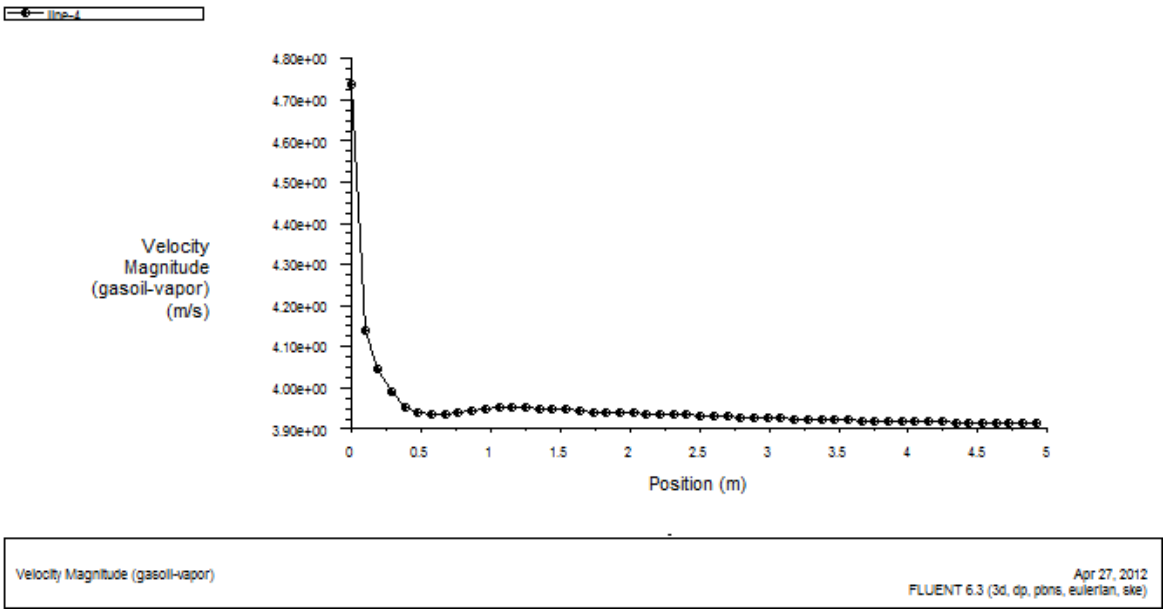


Figure 10: Velocity profile of gas phase

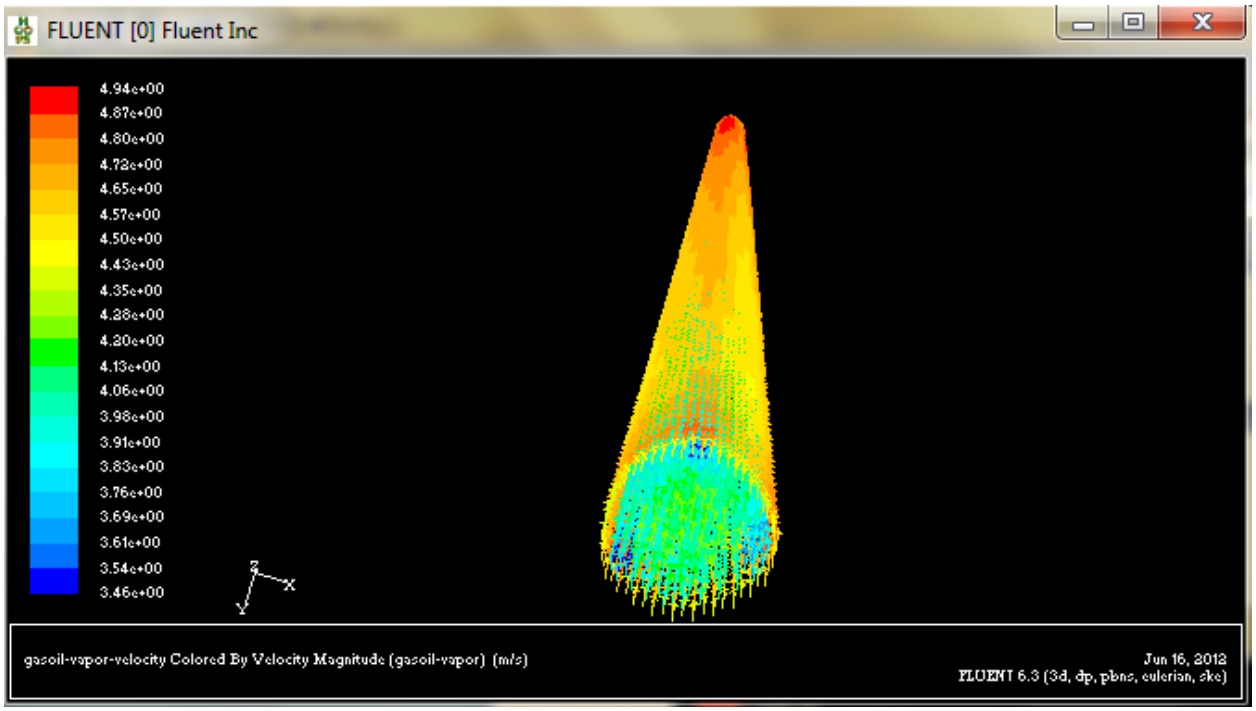


Figure 11: Contour of gas phase velocity

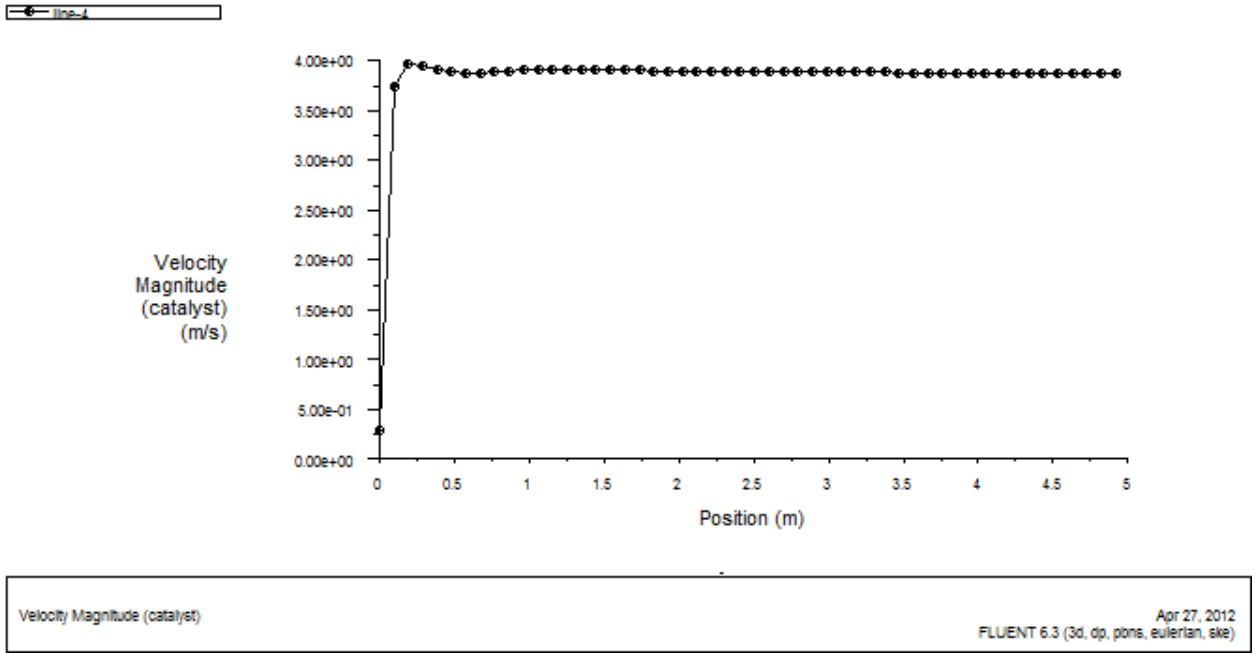


Figure 12: Velocity profile of catalyst phase

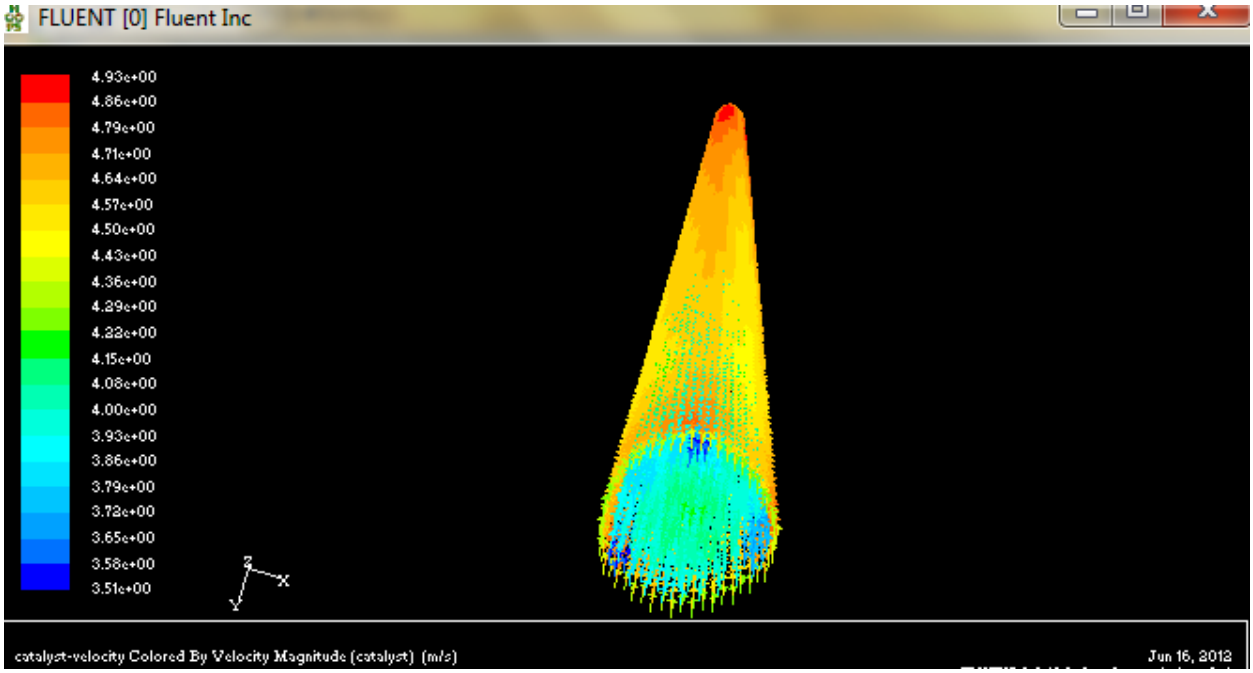


Figure 13: Contour of catalyst phase velocity

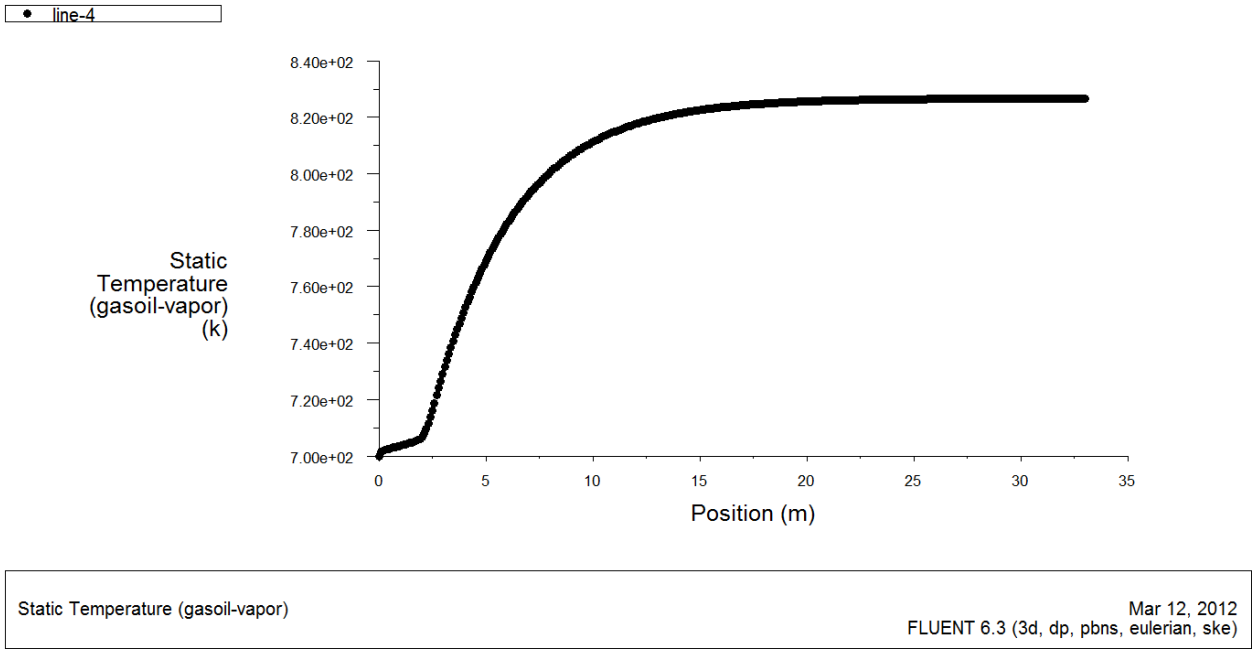


Figure 14: Temperature profile of gas phase

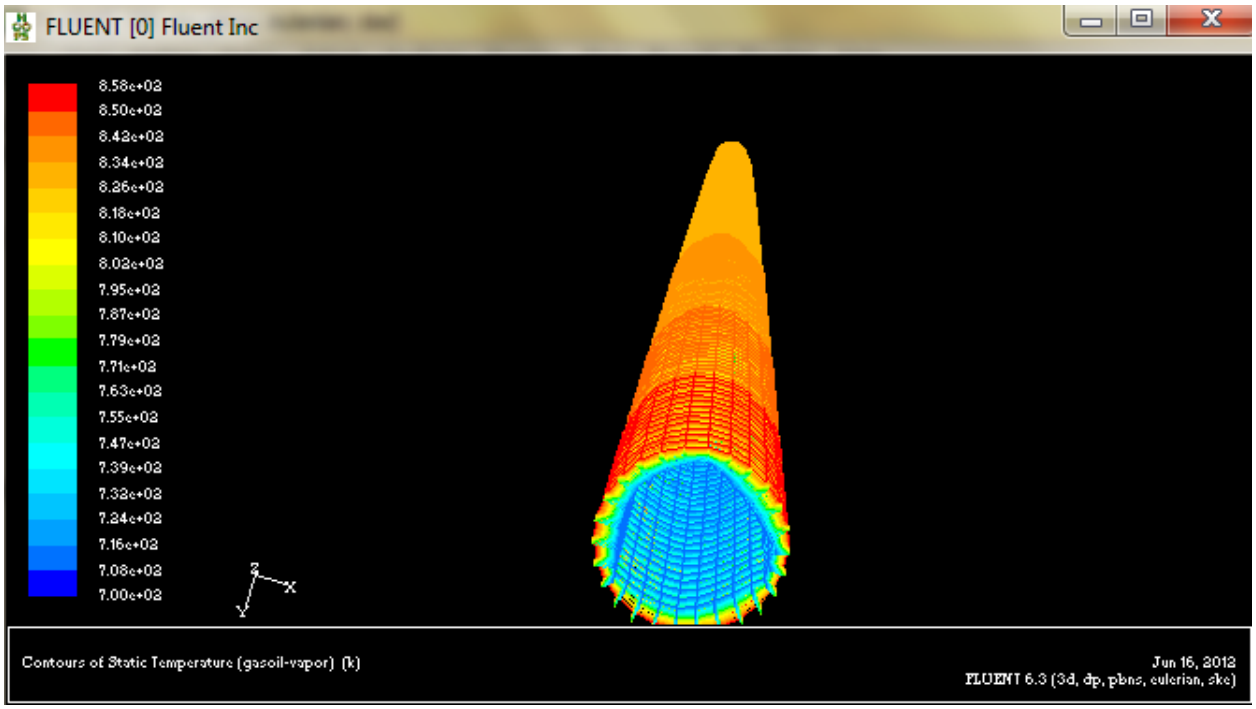


Figure 15: Contour of gas phase temperature

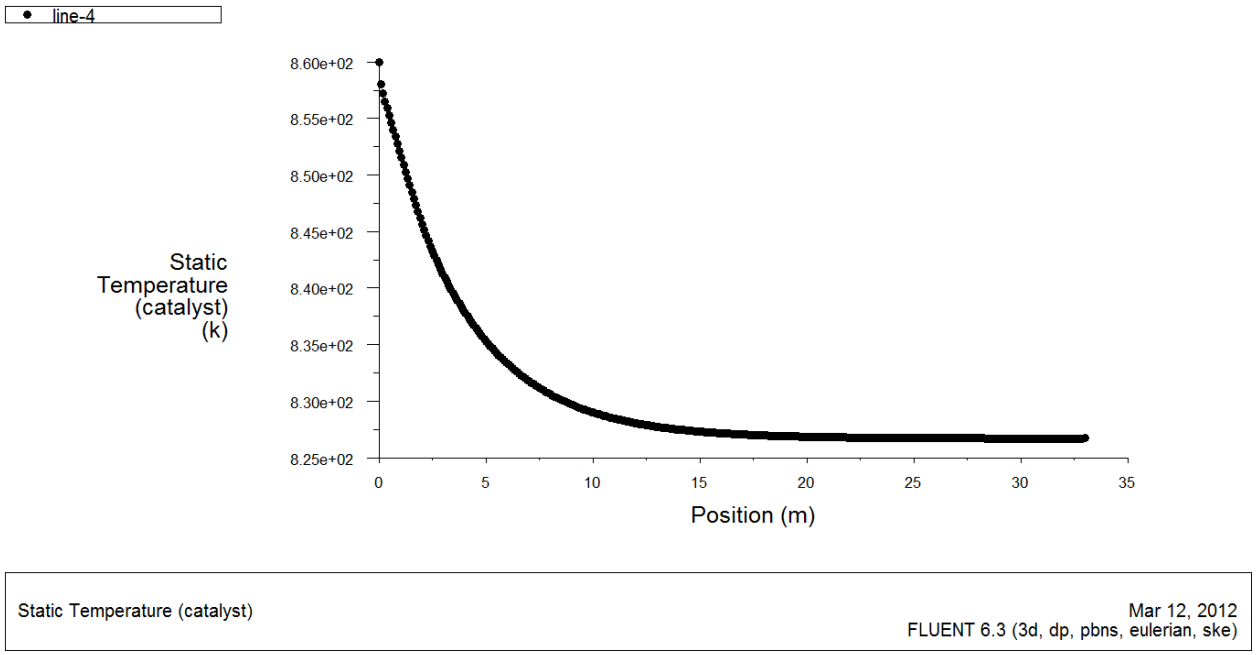


Figure 16: Temperature profile of catalyst phase

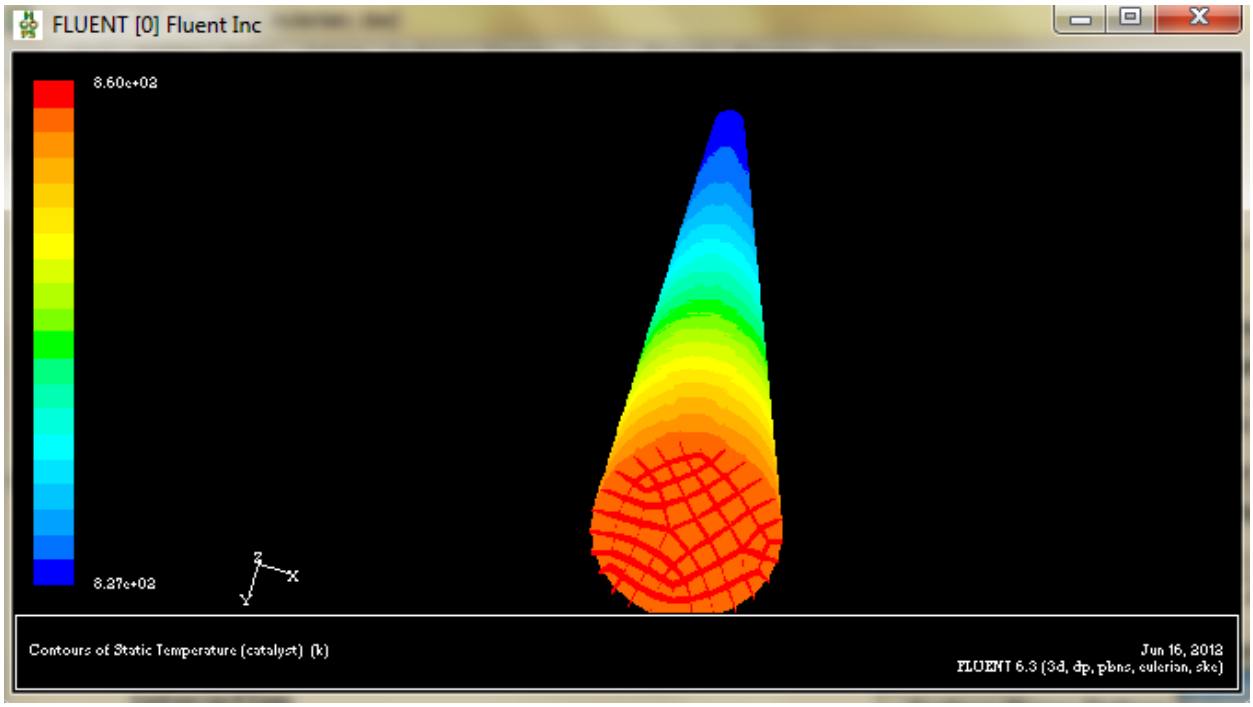


Figure 17: Contour of catalyst phase temperature

Case 2

Further simulations were done on gas-solid flow with reaction. The results obtained are discussed below.

Due to the cracking reactions, the density of the gas phase decreases which results in the increase in gas phase velocity (Figures 18 & 19). Though the catalyst is being dragged by the gas, there is net increase in velocity due to cracking. It can be seen from the contour of velocity magnitude of gas phase (Figure 19) that the velocity keeps on increasing all along the riser height. The feed vapor drags catalyst particles up the riser and there is increase in the velocity of the catalyst along the riser height (Figures 20 & 21).

The heat is transferred from catalyst phase to gas phase. The temperature of gas phase (Figures 22 & 23) increases due to heat gain, and solid phase temperature (Figures 24 & 25) decreases due to heat loss.

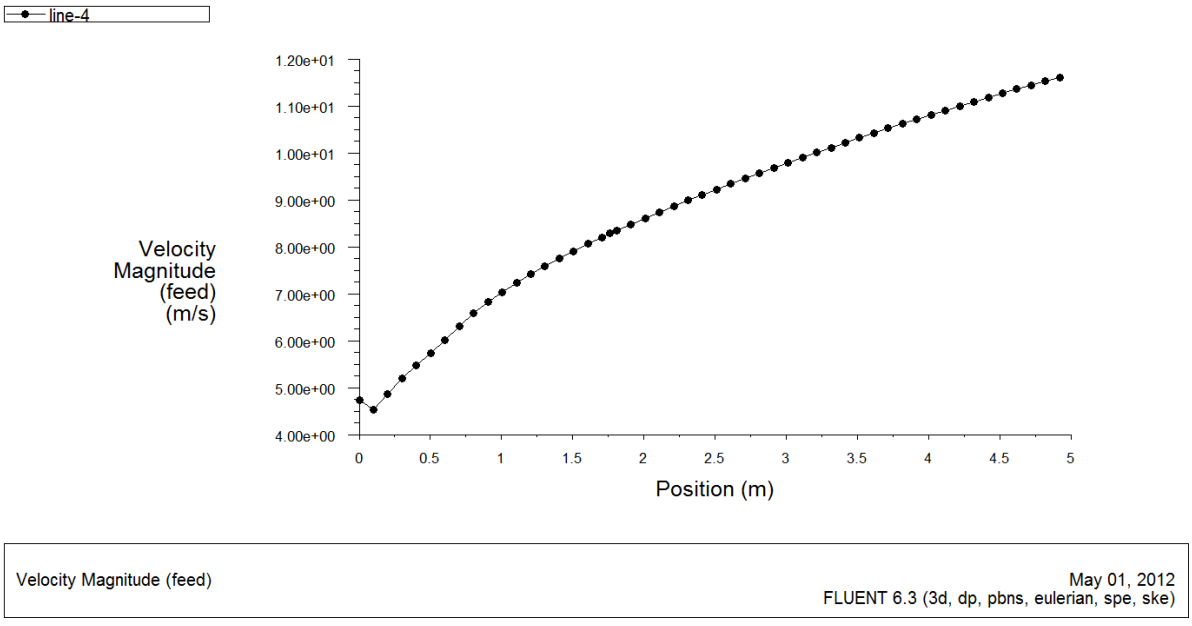


Figure 18: Velocity profile of gas phase

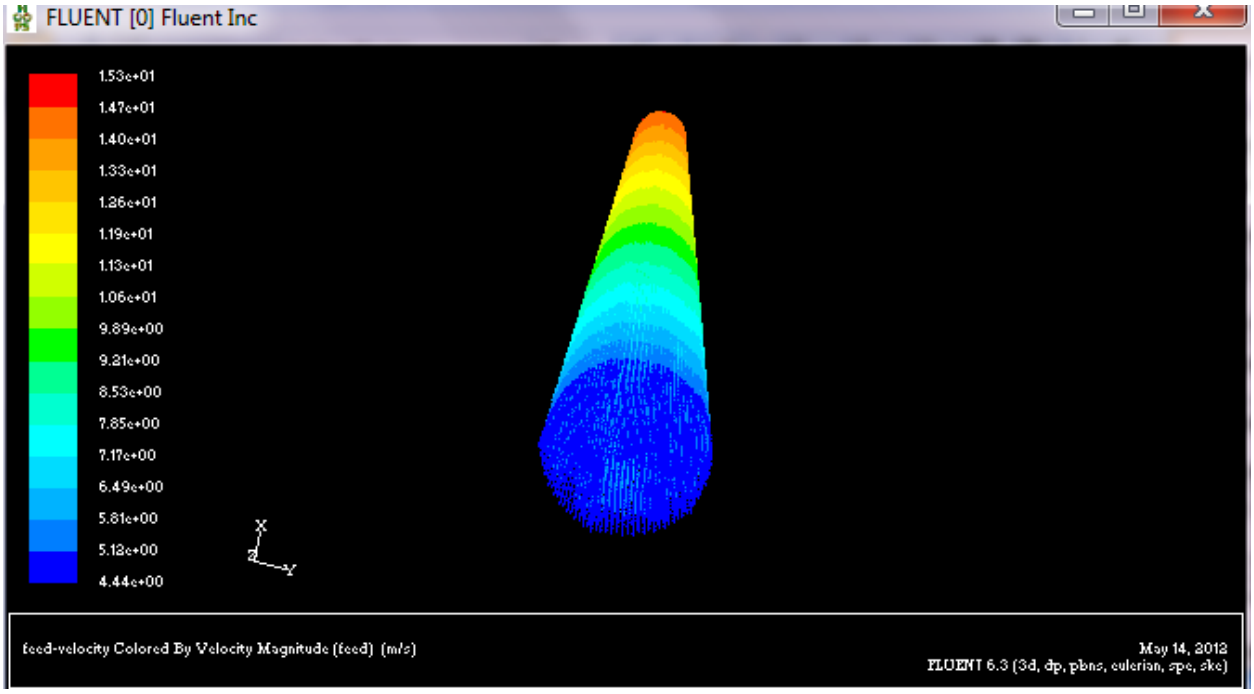


Figure 19: Contour of gas phase velocity

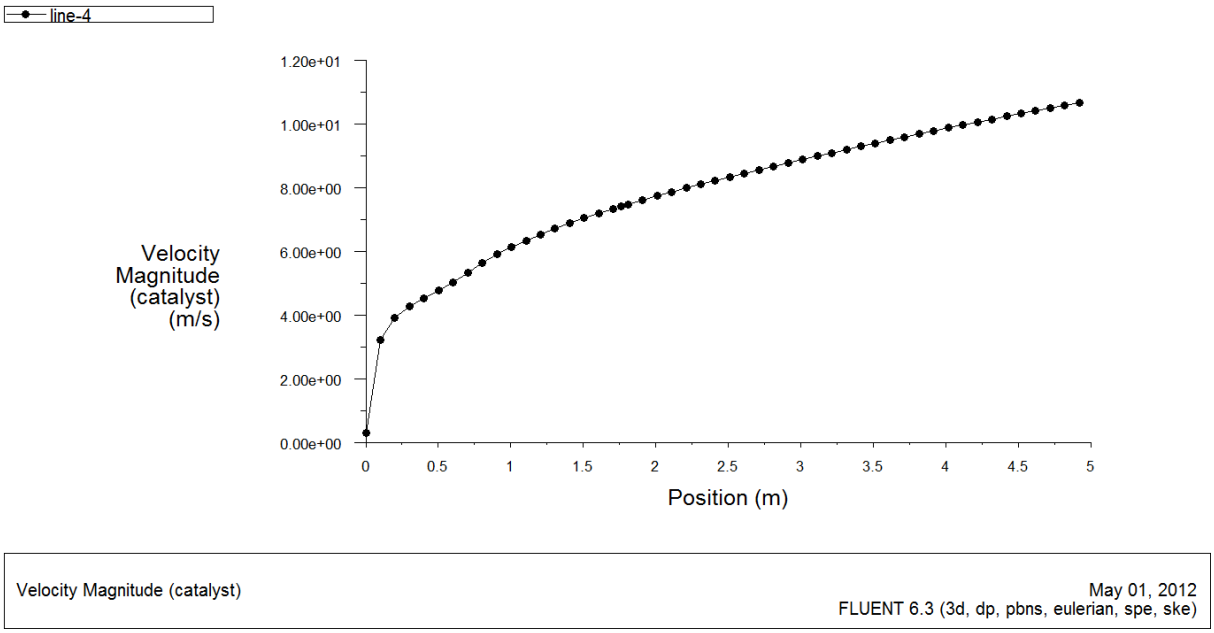


Figure 20: Velocity profile of catalyst phase

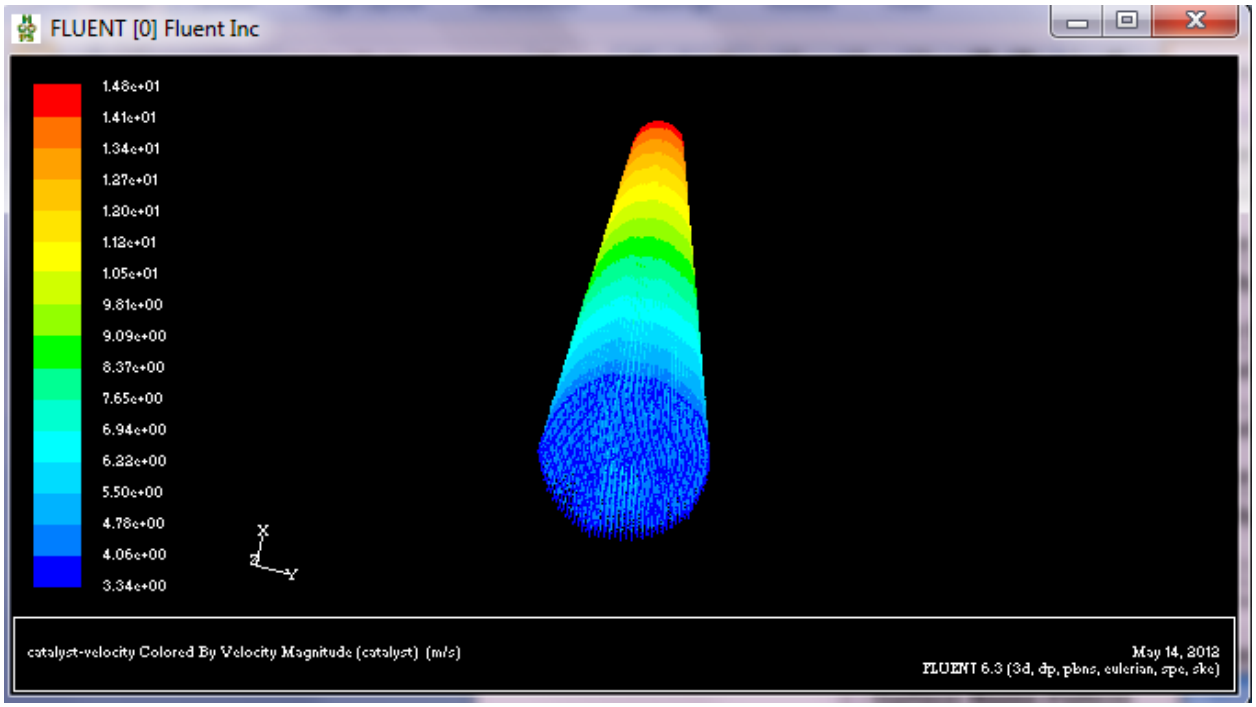


Figure 21: Contour of catalyst phase velocity

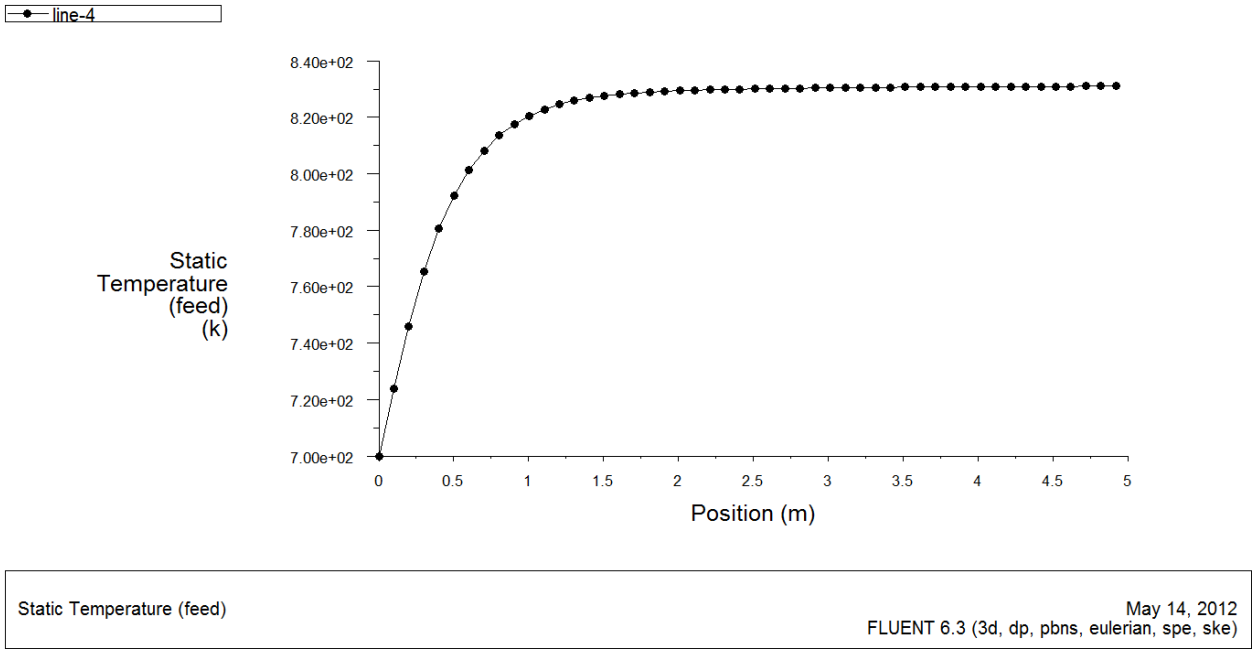


Figure 22: Temperature profile of gas phase

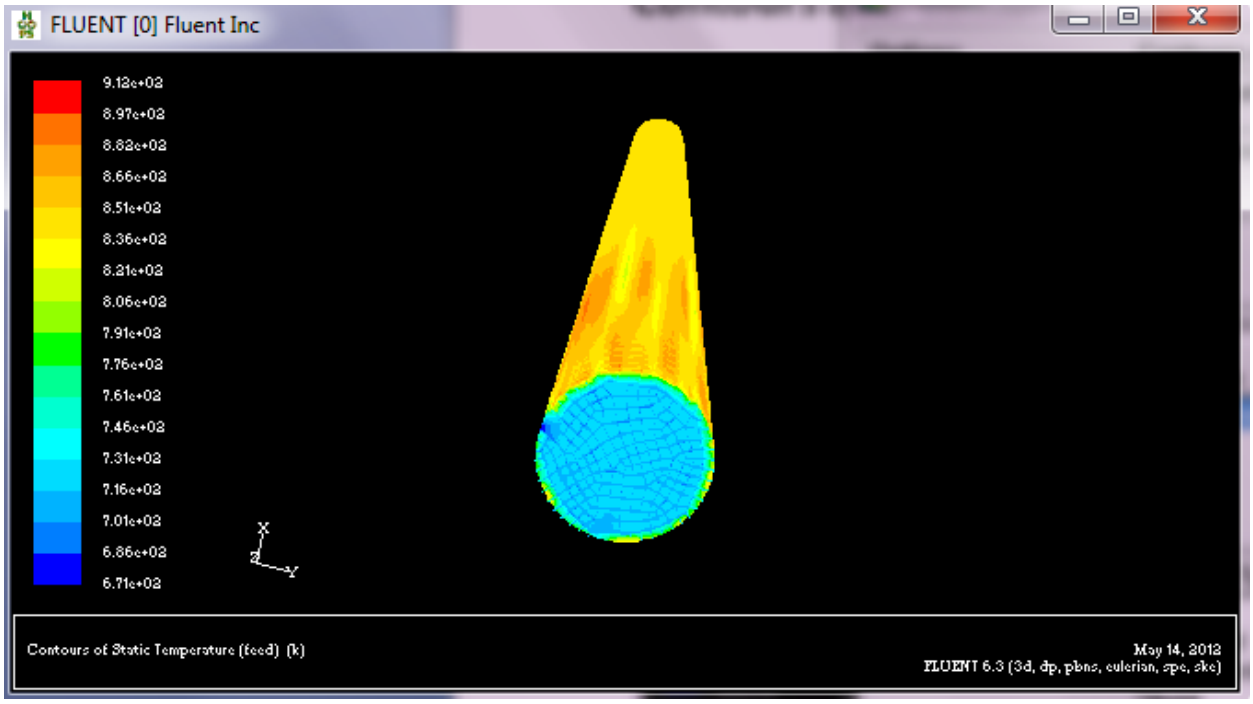


Figure 23: Contour of gas phase temperature

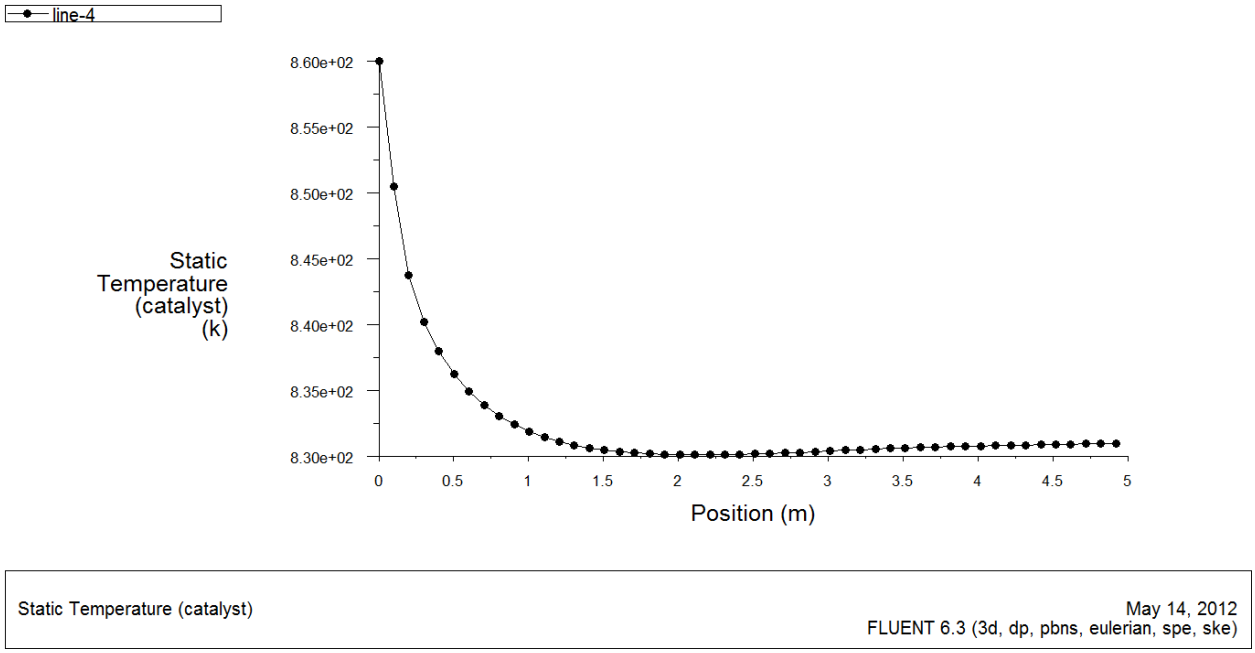


Figure 24: Temperature profile of catalyst phase

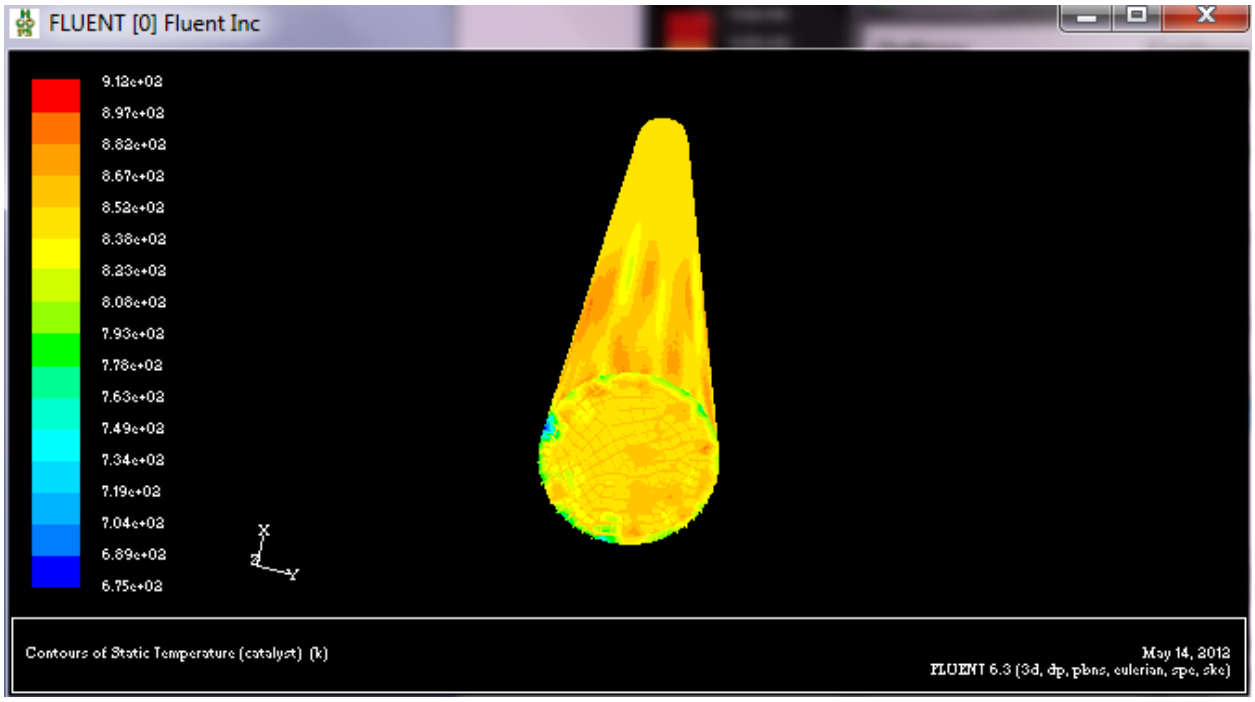


Figure 25: Contour of catalyst phase temperature

The cracking reaction takes place in the riser reactor. The gas-oil cracks to give gasoline, light gases and coke as per the assumed reaction mechanism. The yield is expressed in terms of weight percent. Yields of various products are presented in Table 4. The predicted gas-oil conversion is 62%. The contours of fraction yield of gas-oil, gasoline, light-gases and coke are shown in Figures 26-29.

Table 4 Product Yields

Product	Product yield (wt %)
Gasoline	39
Light –gases	20
Coke	3

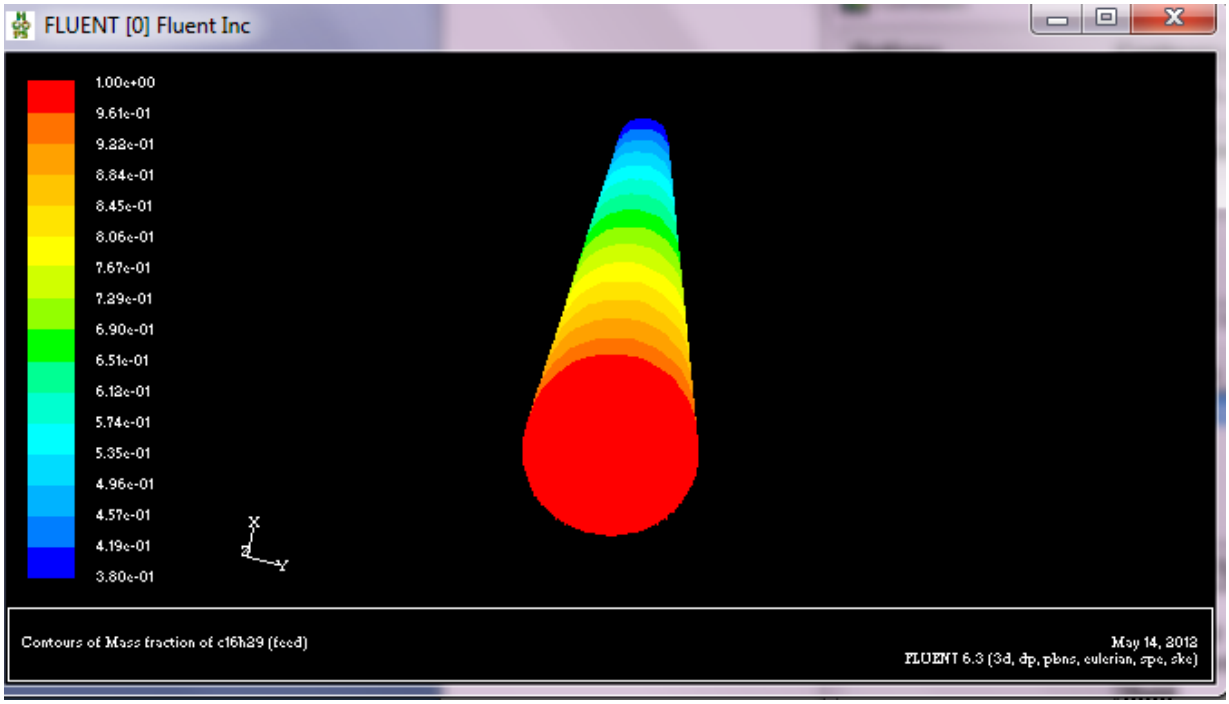


Figure 26: Contour of gas-oil fractional yield along riser height

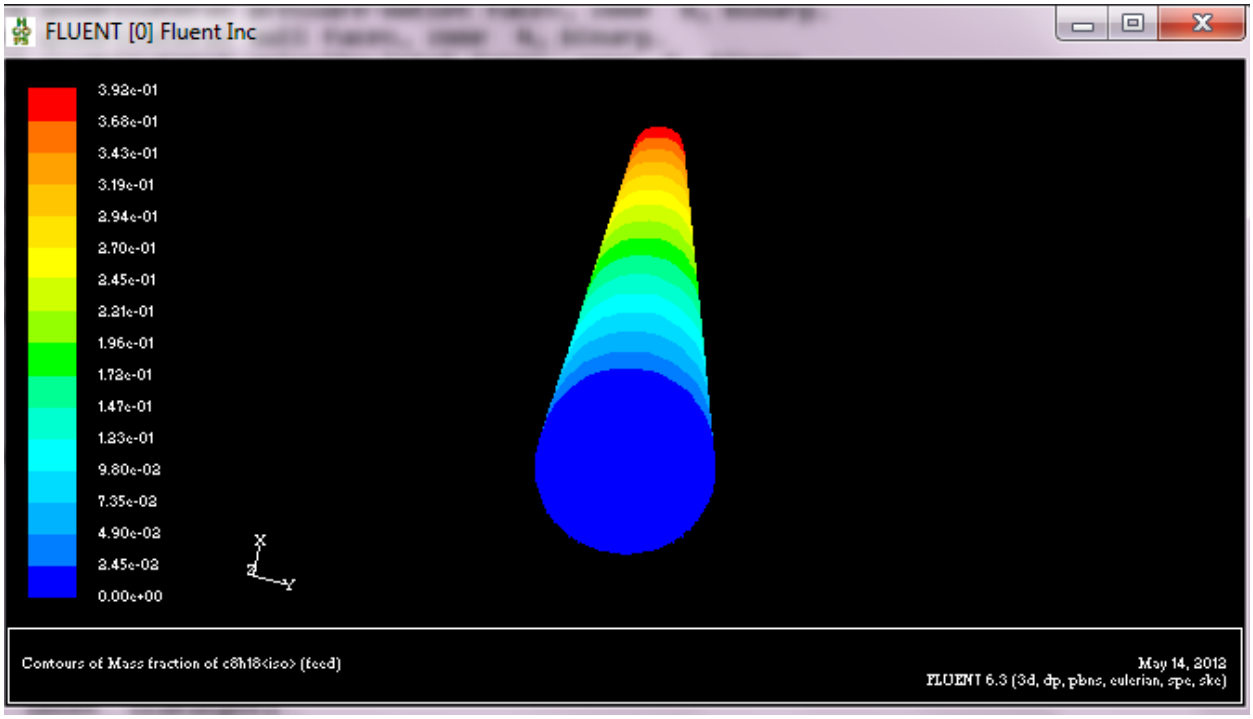


Figure 27: Contour of gasoline fractional yield along riser height

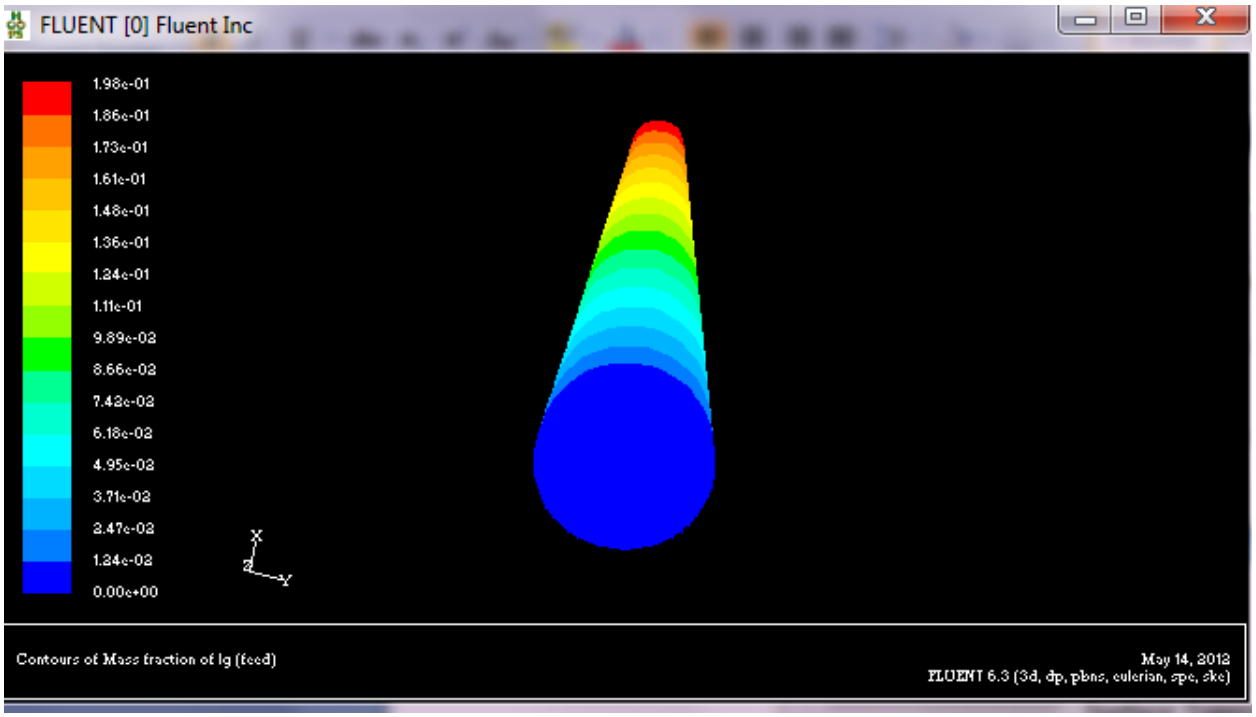


Figure 28: Contour of light-gases fractional yield along riser height

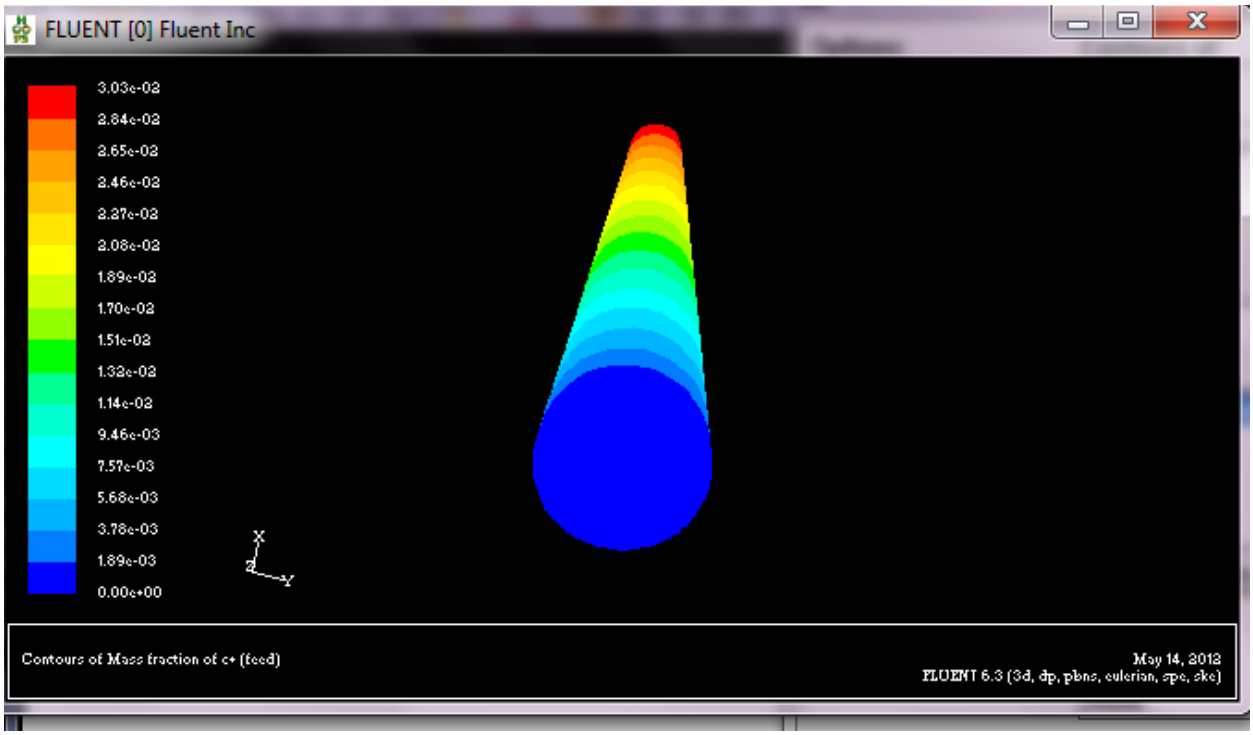


Figure 29: Contour of coke fractional yield along riser height

Contours of reaction rates are shown in Figures 30-34. Near entrance region the rates of gas oil cracking to gasoline, light gases, and coke are high. The cracking rates decrease as gas oil concentration falls along the riser height (Figures 30-32). The gasoline concentration is increasing along the riser height. The contours of gasoline cracking reactions (Figures 33 & 34) show the gasoline cracking rates are increasing along the riser height as the gasoline concentration is increasing.

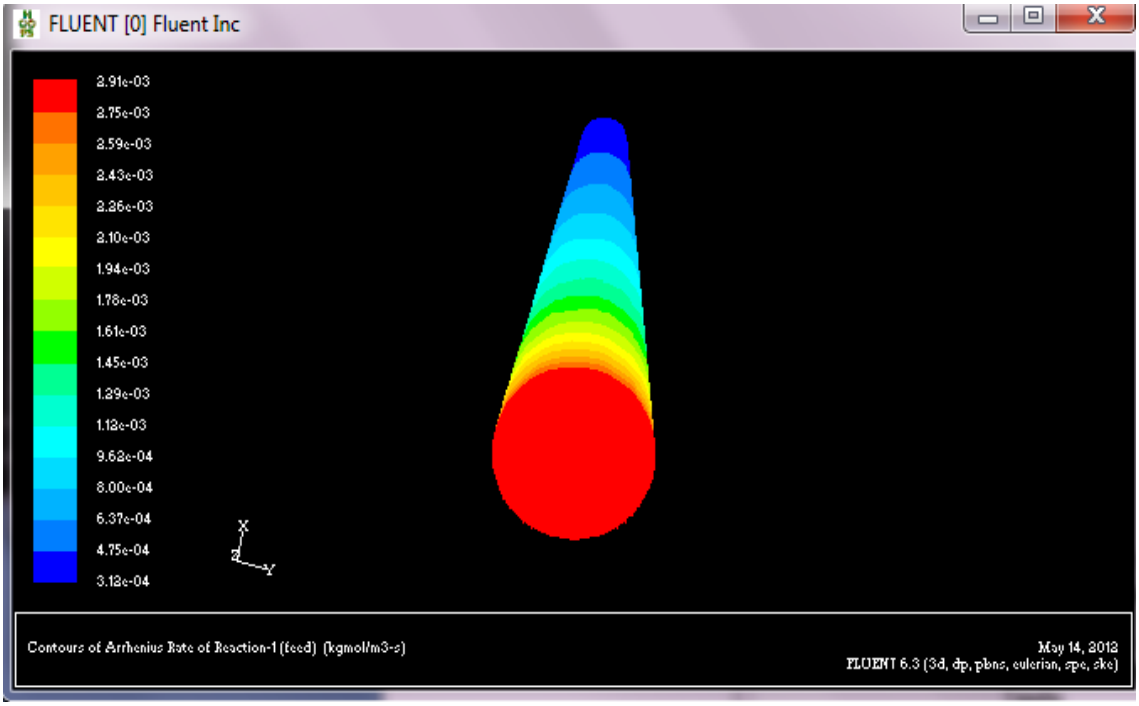


Figure 30: Contour of reaction rate of gasoil cracking to gasoline

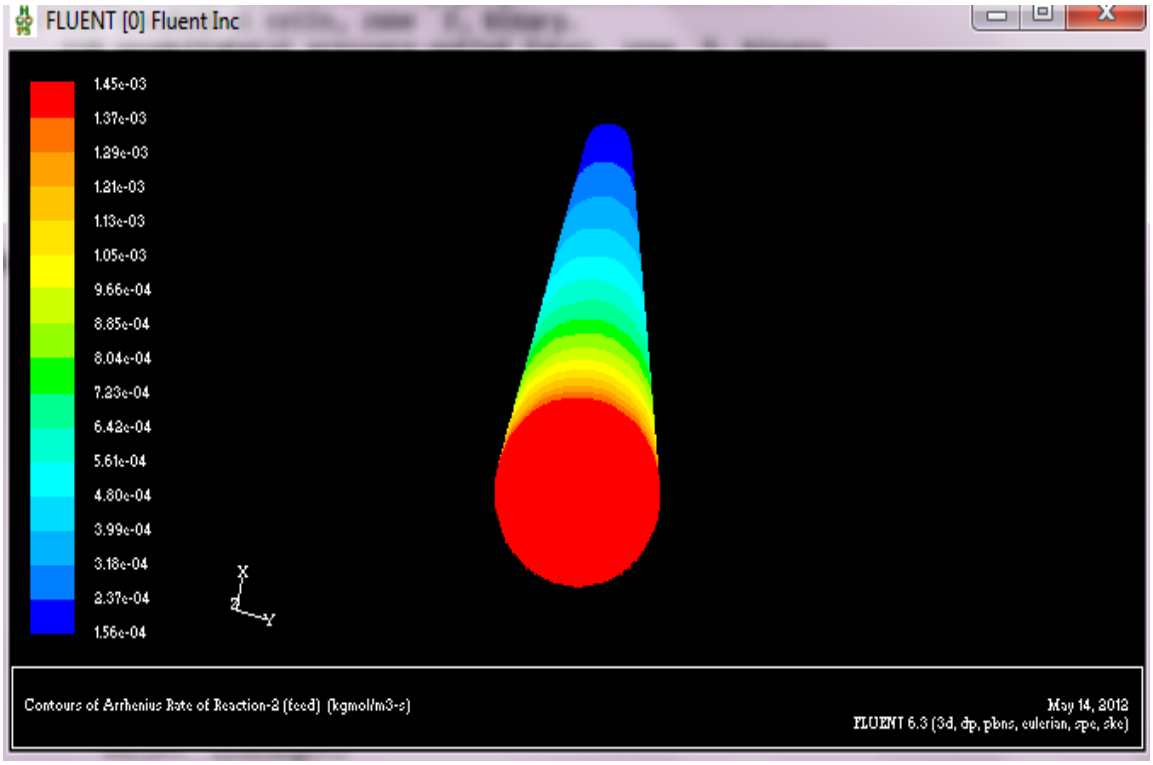


Figure 31: Contour of reaction rate of gasoil cracking to light gases

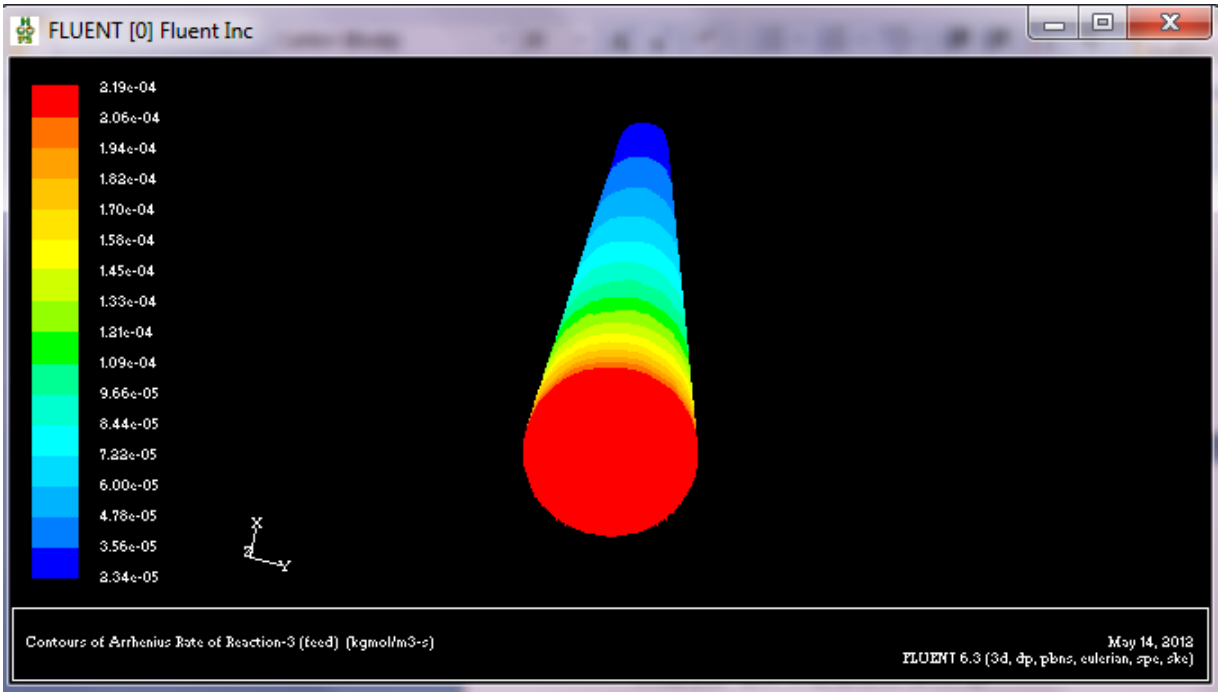


Figure 32: Contour of reaction rate of gasoil cracking to coke

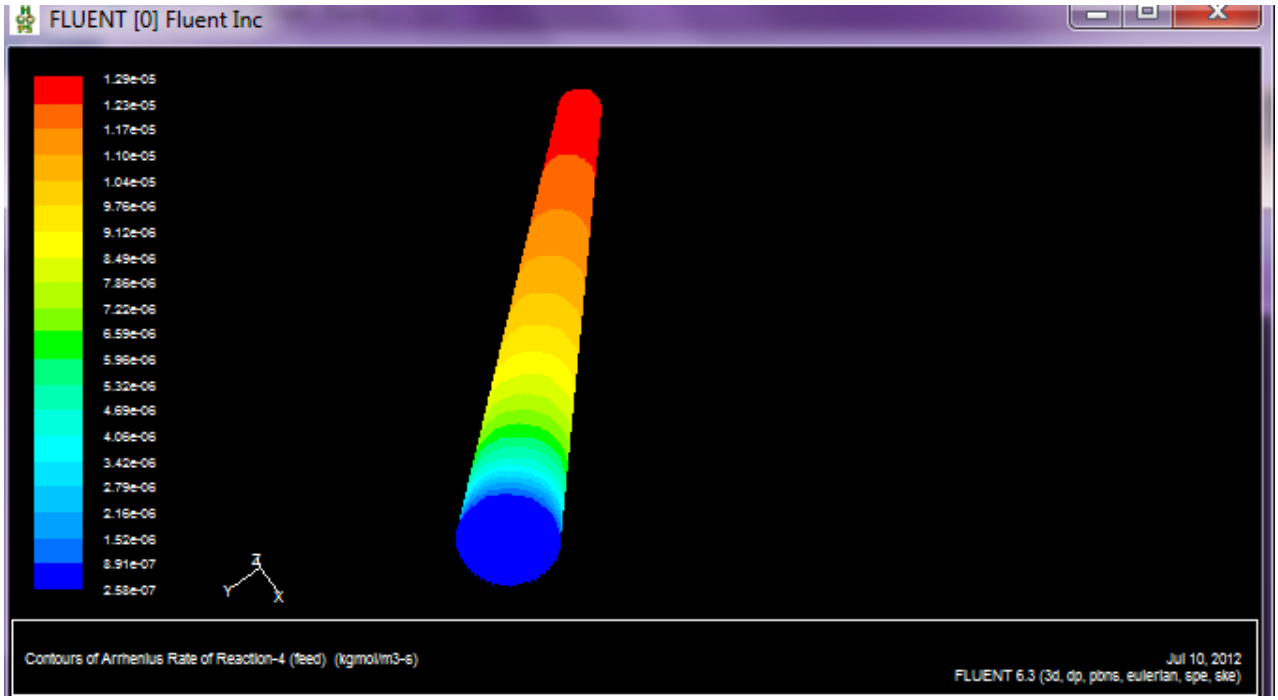


Figure 33: Contour of reaction rate of gasoline cracking to light gases

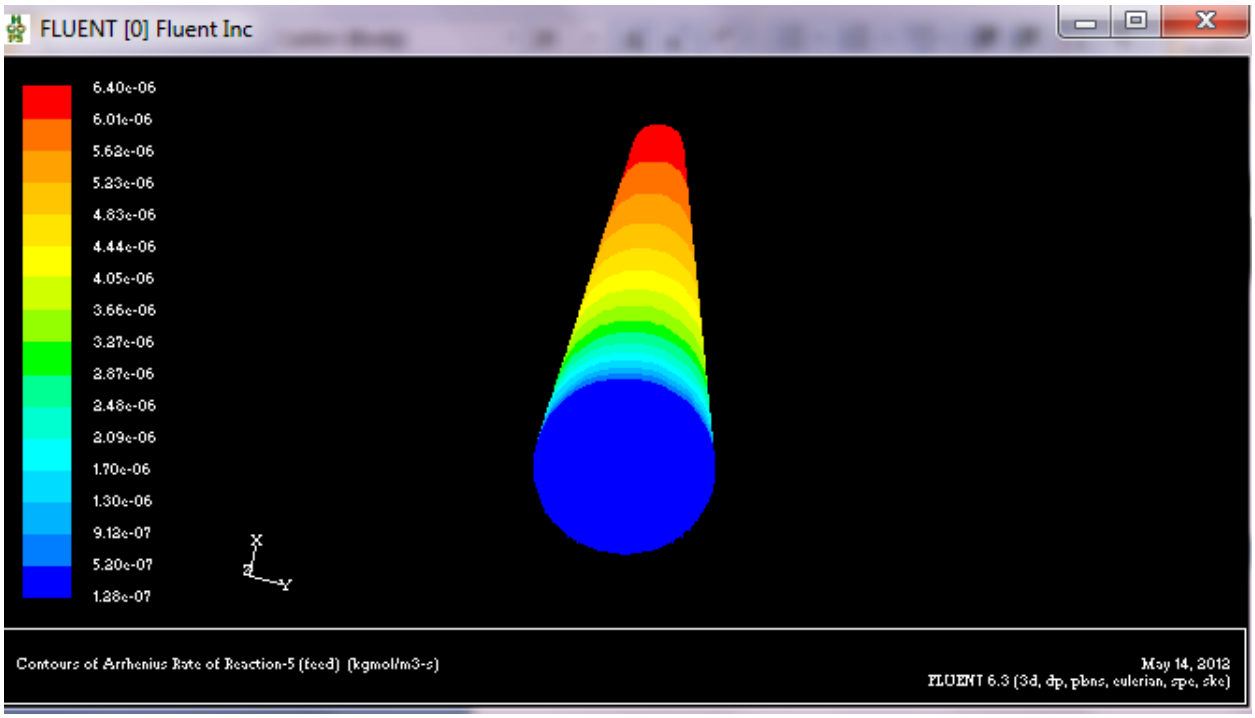


Figure 34: Contour of reaction rate of gasoline cracking to coke

CONCLUSIONS AND FUTURE RECOMMENDATIONS

Conclusions

A model of FCC riser having two phase flow (gas-solid) and a four lump kinetic scheme is simulated using the Eulerian- Eulerian multiphase CFD model. The simulation results of two phase flow model without reaction showed decrease in gas velocity and increase in catalyst velocity. The simulation results of the model when reactions were imposed showed increase in catalyst and gas velocities all along the riser height. The temperature profiles obtained for both the cases were on expected lines.

For gas-solid flow with reaction model the gas phase velocity increased from 4.7 to 14.7 from riser inlet to outlet due to cracking of heavy gas oil to lighter products. The results predicted gas oil conversion 62%, gasoline yield 39%, light gases yield 20%, and coke yield 3%.

Future recommendations

The CFD simulations capabilities for FCC riser modeling can be fully utilized through user defined functions (UDF). The various kinetic models can be implemented in CFD through UDFs for their qualitative and quantitative prediction abilities.

. NOMENCLATURE

C_i	Molar concentration of component i [kmol m^{-3}]
C_d	Drag Coefficient [-]
C_G	Constant of elasticity modulus function [Pa]
C_μ	Constant, 0.09
$C_{\epsilon,1}$	Constant, 1.44
$C_{\epsilon,2}$	Constant, 1.92
d	Particle diameter [m]
E	Activation Energy [J mol^{-1}]
g	Gravitational acceleration [$m^2 s^{-1}$]
G	Elasticity modulus
H	Static enthalpy [J mol^{-1}]
k_r	Kinetic constant of reaction [$m^3 kmol^{-1} s^{-1}$]
K	turbulent kinetic energy [$m^2 s^{-2}$]
k_r^0	Pre-exponential factor [$m^3 kmol^{-1} s^{-1}$]
Nu	Nusselt number [-]
p	Static pressure [Pa]
P^k	Shear production of turbulence [Pa s^{-1}]
Pr	Prandtl number [-]
Re	Reynolds number [-]
T	Static temperature [K]

u	Velocity vector [m s^{-1}]

Greek letters

β	Interphase momentum transfer [kg $m^{-3}s^{-1}$]
ε	Volume fraction [-]
ϵ	Turbulence dissipation rate [m^2s^{-3}
γ	Interphase heat transfer coefficient [$Wm^{-2}K^{-1}$]
Γ	Diffusivity [$kgm^{-1}s^{-1}$]
λ	Thermal conductivity [$Wm^{-1}K^{-1}$]
μ	Molecular viscosity [Pa s]
ρ	Density [kgm^{-3}]
σ_k	Constant, 1.00
σ_ϵ	Constant, 1.30

Subscripts

g	Gas phase
s	Solid phase
R	Reaction
lam	Laminar
turb	turbulent

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