

MODELING AND SIMULATION FOR FCC UNIT FOR THE ESTIMATION OF GASOLINE PRODUCTION

Sreshtha G. Bhende and Kiran D. Patil*

Department of Petroleum and Petrochemical Engineering,
Maharashtra Institute of Technology, Paud Road, Kothrud, Pune-411 038, India

* Author for correspondence: kiran.patil@mitpune.edu.in, Tel: +91-20-30273512, Fax: +91-2025442770

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ABSTRACT

Fluid catalytic cracking (FCC) is one of the most important processes in the petroleum refining industry for the conversion of heavy gas oil to gasoline and diesel. Furthermore, valuable gases such as ethylene, propylene and isobutylene are produced. This work describes development of a mathematical model that can simulate the behavior of the FCC unit, which consists of feed and preheat system, riser, stripper, reactor, regenerator, and the main fractionator. The model describes the seven main sections of the entire FCC unit: (1) the feed and preheating system, (2) riser, (3) stripper, (4) reactor, (5) regenerator, and (6) main fractionator. This model is able to predict and describe the compositions of the final production rate, and the distribution of the main components in the final product. This allows the estimation of economic factors, related to the operation of the FCCU. For the present study, a refinery process is simulated in Aspen Hysys v7.3 environment. Simulation Basic Manager, a fluid package is selected along with the components which are to be in the input stream. In the process, Peng-Robinson was selected as the fluid package as it is able to handle hypothetical components (pseudo-components). In this work, a basic refinery process is designed and the vacuum gas oil from the vacuum distillation column is used as feed in the FCC unit.

Keywords: FCC unit, Mathematical modeling, Aspen Hysys, Simulation, catalyst, riser.

I. INTRODUCTION:

An oil refinery or petroleum refinery is an industrial process plant where crude oil is processed and refined into more useful products such as petroleum naphtha, gasoline, diesel fuel, asphalt base, heating oil, kerosene, and liquefied petroleum gas. Oil refineries are typically large, sprawling industrial complexes with extensive piping running throughout, carrying streams of fluids between large chemical processing units.[1] An oil refinery is considered an essential part of the downstream side of the petroleum industry. Fluid catalytic cracking (FCC) continues to play a key role in an integrated refinery as the primary conversion process. For many refiners,

the cat cracker is the key to profitability in that the successful operation of the unit determines whether or not the refiner can remain competitive in today's market. Approximately 350 catalytic crackers are operating worldwide, with a total processing capacity of over 12.7 million barrels per day. Most of the existing FCC units have been designed or modified by six major technology licensors out of whom the most used is by UOP. [1]

The FCC process is very complex. The FCC unit uses a microspheroidal catalyst, which behaves like a liquid when properly aerated by gas. The common objective of these various FCC units is to upgrade low-value feedstock to more valuable

products. The main purpose of the unit is to convert high-boiling petroleum fractions called gas-oils to high value, high-octane gasoline and heating oil. Since the start-up of the first commercial FCC unit in 1942, many improvements have been made. These improvements have enhanced the unit's mechanical reliability and its ability to crack heavier, lower value feedstock. The FCC has a remarkable history of adapting to continual changes in market demands.

[II] LITERATURE REVIEW:

The basic process of FCC has got two major components i.e. reactor and regenerator. The feed in the FCC riser are the residue and the Atmospheric gas oil which comes out from the distillation column. The feed needs to be preheated before entering in the riser part. This is done by the feed preheat system which heats both the fresh and recycled feed through several heat exchangers and the temperature is maintained at about 500-700°F. The gas oil consists of paraffinic, aromatics and naphthenic molecules and also contains various amounts of contaminants such as Sulphur, nitrogen which have detrimental effect on the catalyst activity. Hence, in order to protect the catalyst feed pre-treatment is essential which removes the contaminants and have better cracking ability thus giving higher yields of naphtha. The riser is the main reactor in which most of the cracking reactions occur and all the reactions are endothermic in nature.

The residence time in the riser is about 2–10 s. At the top of the riser, the gaseous products flow into the fractionator, while the catalyst and some heavy liquid hydrocarbon flow back in the disengaging zone. Steam is injected into the stripper section, and the oil is removed from the catalyst with the help of some baffles installed in the stripper. The earlier practice of carrying out the cracking reactions in the reactor has now been completely replaced by carrying out it in the riser part. This is done to utilize the maximum catalyst activity and temperature inside the riser. Earlier, no significant attempts were made for controlling the riser operations.

[3] But after the usage of the reactive zeolite catalyst the amount of cracking occurring in the riser has been enhanced. Now the reactor is used for the separation purpose of both the catalyst and the outlet products. Reactions in the riser are optimized by increasing the regenerated catalyst velocity to a desired value in the riser reactor and injecting the feed into the riser through spray nozzles.

The main purpose of reactor is to separate the spent catalyst from the cracked vapors and the spent catalyst flows downward through a steam stripping section to the regenerator. The cracking reaction starts when the feed is in contact with the hot catalyst in the riser and continues until oil vapors are separated from the catalyst in the reactor separator. The hydrocarbons are then sent to the fractionator for the separation of liquid and the gaseous products. In the reactor the catalyst to oil ratio has to be maintained properly because it changes the selectivity of the product.

The catalyst's sensible heat is not only used for the cracking reaction but also for the vaporization of the feed. During simulation the effect of the riser is presumed as plug flow reactor where there is minimal back mixing, but practically there are both downward and upward slip due to drag force of vapour.[4] The spent catalyst coming out from steam stripping section goes in the regenerator.

Regenerator maintains the activity of the catalyst and also supplies heat to the reactor. Depending upon the feed stock quality there is deposition of coke on the catalyst surface. To reactivate the catalyst, air is supplied to the regenerator by using large air blowers. High speed of air is maintained in the regenerator to keep the catalyst bed in the fluidized state. Then through the distributor at the bottom air is sent to the regenerator. Coke is burned off during the process in significant amount. The regenerator operates at a temperature of about 715 °C and a pressure of about 2.41 bars. The hot catalyst (at about 715 °C) leaving the regenerator flows into a catalyst where any flue gases are allowed to escape and flow back into the upper part to the regenerator.

The flow of the regenerated catalyst is regulated by a slide valve in the regenerated catalyst line. The hot flue gas exits the regenerator after passing through multiple sets of two-stage cyclones that removes entrained catalyst from the flue gas. The heat is produced due to the combustion of the coke and this heat is utilized in the catalytic cracking process. Heat is carried by the catalyst as sensible heat to the reactor. Flue gas coming out of the regenerator is passed through the cyclone separator and the residual catalyst is recovered.

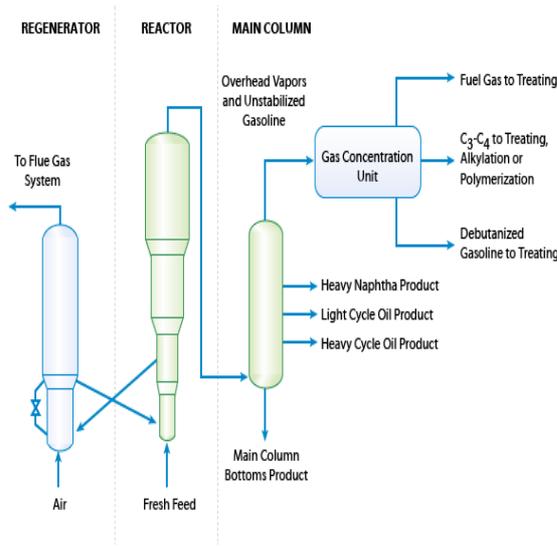


Figure 1: Typical UOP type FCC unit.

The specification of the catalyst will be discussed in detail at literature review. The regenerator is designed and modeled for burning the coke into carbon monoxide or carbon dioxide. Earlier, conversion of carbon to carbon monoxide was done which required lesser air supply hence the capital cost was reduced.[4] But now a day's air is supplied in such a scale that carbon is converted into carbon dioxide in this case the capital cost is higher but the regenerated catalyst has minimum coke content on it.

The flue gases like carbon monoxide are burned off in a carbon monoxide furnace (waste heat boiler) to carbon dioxide and the available energy is recovered. The hot gases can be used to generate steam or to power expansion turbines to compress the regeneration air and generate power. There are two stage cyclones which

remove any entrained catalyst from the flue gases.

[III] ANALYTICAL MATHEMATICAL MODELING:

In current refineries, the FCC unit plays a prominent role, producing gasoline and diesel, as well as valuable gases, such as ethylene, propylene and isobutylene, from feedstocks that comprise atmospheric gas oils, vacuum gas oils and hydrocracker bottoms.[2] The significant economic role of the FCC unit in modern-day petroleum refining has attracted great interest in academia and industry in terms of developing and modeling control algorithms for efficient FCC application. The main parts of the FCC unit that have been modeled are riser, reactor and fractionator.

The riser of the FCC unit is assumed to be a reactor in which all the complex reactions take place. Since maximum conversion takes place in riser it was assumed to be a conversion reactor where in mass transfer takes place.[2] For simplicity, we will assume isothermal, constant-holdup, constant-pressure, and constant density conditions and a perfectly mixed liquid phase. The total mass-transfer area of the bubbles is A and it could depend on the gas feed rate FA . A constant-mass-transfer coefficient: $t k$, (with units of length per time) is used to give the flux of A into the liquid through the liquid film as a function of the driving force.

$$N_A = k_L (C_A^* - C_1) \tag{1}$$

Mass transfer is usually limited by diffusion through the stagnant liquid film because of the low liquid diffusivities.

We will assume the vapour-phase dynamics are very fast and that any unreacted gas is vented off the top of the reactor. So we can write,

$$F_V = F_A - (A_{MT} N_A M_A) / P_A \tag{2}$$

Component continuity for A :

$$V (d C_A / dt) = A_{MT} N_A - F_L C_A - V k C_A C_B \tag{3}$$

Component continuity for B:

$$V (d C_B / dt) = F_B C_{B0} - F_C C_B - V k C_A C_B \tag{4}$$

Total continuity:

$$d(\rho V)/dt = 0 = F_B \rho_B + M_A N_A A_{MT} - F_L \rho \quad (5)$$

The reactor of the FCC unit is assumed to be a constantly-stirred tank reactor (CSTR) which operates under pressure. The outflow will vary with the pressure and the composition of the reactor. Density varies with pressure and composition.[6]

$$F = C \sqrt{\frac{P - PD}{\rho}} \quad (6)$$

$$\tilde{n} = MP/RT = \{[yM_A + (1-y) M_B]P\}/RT \quad (7)$$

Where, C_v =valve sizing coefficient,
 M =average molecular weight,
 M_A = molecular weight of the reactants,
 M_B = molecular weight of the products.

Total continuity:

$$V (dp/dt) = \rho_o F_o - Pp \quad (8)$$

The fractionator of the FCC unit is modeled as a multi-component non-ideal distillation column. The assumptions that we will make are, liquid on the tray is perfectly mixed and incompressible, tray vapour holdups are negligible, dynamics of the condenser and the reboiler will be neglected and vapour and liquid are in thermal equilibrium (same temperature) but not in phase equilibrium. A Murphree vapour-phase efficiency will be used to describe

the departure from equilibrium. [7]

$$E_{nj} = (y_{nj} - y_{n-1,j}^T) / (y_{nj}^* - y_{n-1,j}^T) \quad (9)$$

Where y_{nj}^* = composition of vapour in phase equilibrium with liquid on n^{th} tray with composition x_{nj} , y_{nj} = actual composition vapour leaving n^{th} tray, $y_{n-1,j}^T$ = actual composition of vapour entering n^{th} tray, E_{nj} = Murphree vapour efficiency for j^{th} component on n^{th} tray.

Total continuity (one per tray):

$$d(M_n)/dt = L_{n+1} + F_n^L + F_{n-1}^V + V_{n-1} - V_n - L_n - S_n^L - S_n^V \quad \dots (10)$$

[IV] SIMULATION:

The above models were developed in Aspen Hysys v7.3 environment. Simulation Basic Manager, a fluid package is selected along with the components which are to be in the input stream. In the process, Peng-Robinson was selected as the fluid package as it is able to handle hypothetical components (pseudo-components).

The non-oil components used for the process were H₂O, CH₄, C₂, C₃, n-C₄, i-C₅, n-C₅ and n-C₁₀. The pseudo-components were created by supplying the data to define the assay. The fluid package contains 25 components (NC: 25). In order to go to the PFD screen of the process the option “Enter to simulation Environment” was clicked on. An object palette appeared at right hand side of the screen displaying various operations and units.

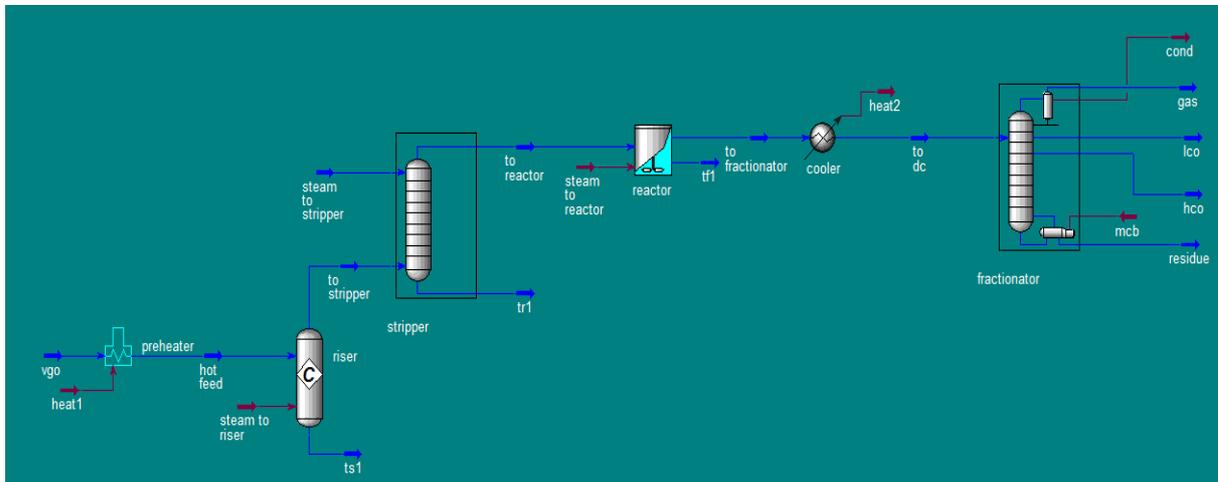


Figure 2: Model of FCC unit in Aspen Hysys

Here the heater's icon was changed and assumed to be pre-heater. The conversion reactor is assumed to be the riser and the constantly-stirred tank reactor as the reactor. The operating data for these equipments inserted is equal to the data on which a normal FCC unit runs in any refinery.

[V] RESULT AND DISCUSSION:

The properties discussed in this section are temperature, pressure, flow rates, light liquid, K-value and transport properties.

(1) Temperature v/s Tray Position:

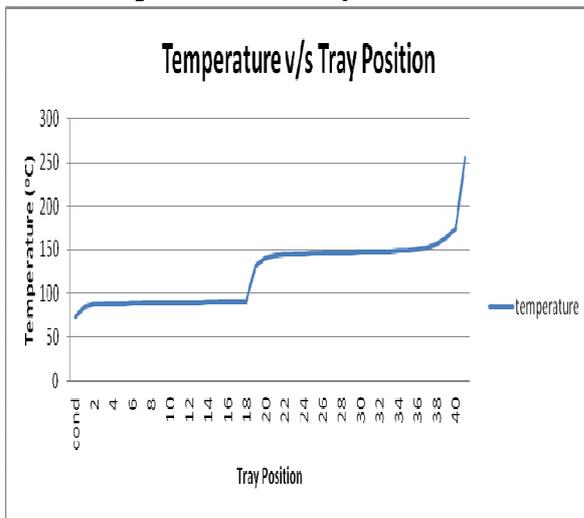


Figure 3: Plot of Temperature v/s Tray Position

Temperature increases from the top to bottom as the position of the tray increases from top to bottom in the fractionator column. This is happening due to the true boiling point (TBP) of the cuts. From this plot we can conclude that the light gaseous cut is obtained from the top of the fractionator column this contains methane, ethane, propane, butane and pentane. From the composition, all the components that have TBP are till 72°C are collected as gas from the top of the fractionator column.

As we proceed downward the liquids become heavy and have tendency to absorb more heat, hence their TBP is higher and hence curve moves steeply upward. Since the TBP of LCO is 115°C, hence at the cut of LCO the temperature of its draw is 92 °C. And hence for HCO the draw temperature is at 145 °C. The residue is collected from the bottom of the fractionator column at 245 °C.

(2) Pressure v/s Tray Position:

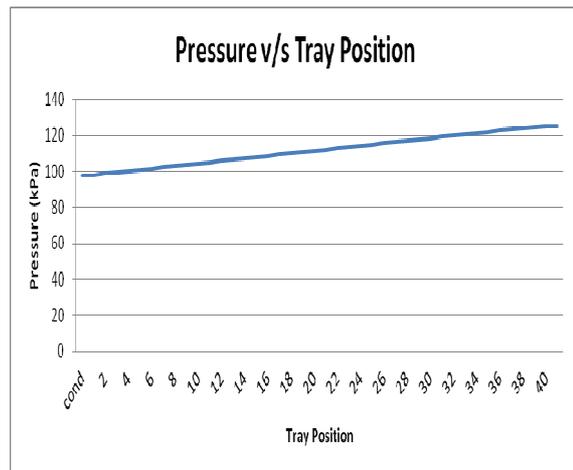


Figure 4: Plot of Pressure v/s Tray position

Usually during the model development we used the unit of pressure as kg/cm², but for this plot, the unit of pressure is in kPa. From the plot it is clear that the pressure increases from top to bottom of the fractionator column. It has same reason as that for the rise in the temperature from top to bottom of the fractionator column.

(3) Flow v/s Tray Position:

From this plot as shown in Figure 5, we can see that on the top section of the column the flow of vapours is more than that of liquids. This means that more of light components are present in vapour phase and hence they are separated from top of the column, from which we can conclude that more of gasoline and LPG can be obtained from the gases separated from the top of the column?

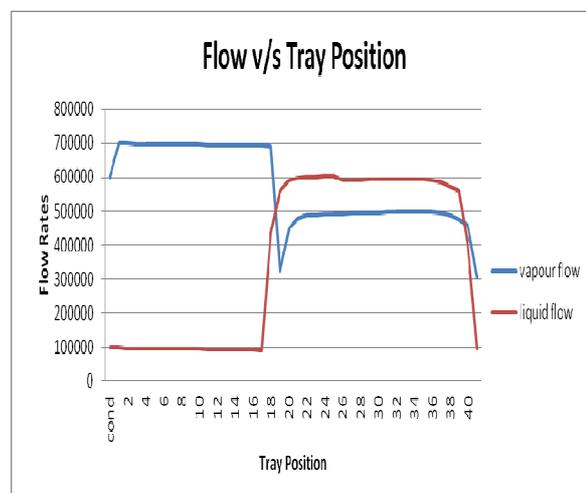


Figure 5: Plot of Flow v/s Tray position

The flow rates within the phases changes almost from where the heavy liquids are drawn off from the fractionator column. But from the plot we see that the flow of vapours almost diminishes to the lower trays. This means the cuts drawn off from the column and the residue obtained are major in liquid phase but also consists some of vapors, hence care needs to be taken during the transportation of these liquids. First the vapour needs to be separated and then the liquid should be transported to the storage tanks.

(4) K-Value v/s Tray Position:

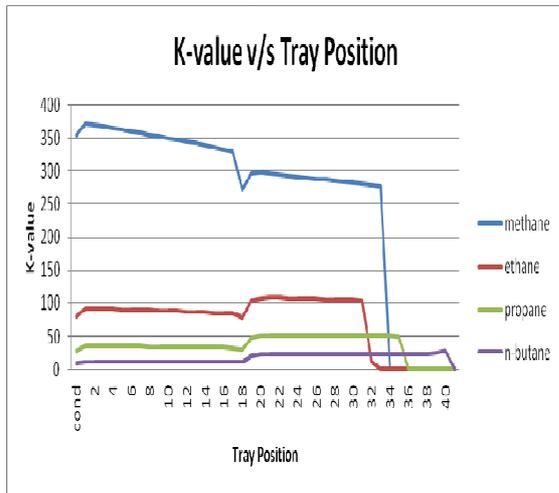


Figure 6: Plot of K-value v/s Tray position

Vapour–liquid equilibrium (VLE) is a condition where a liquid and its vapour (gas phase) are in equilibrium with each other, a condition or state where the rate of evaporation equals the rate of condensation on a molecular level such that there is no net or overall vapour–liquid inter-conversion. A vapour-liquid equilibrium ratio (*K*-value) is defined for a component as the ratio of mole fraction in the vapour to mole fraction in the liquid for that component.

The tendency of a given chemical species to partition itself preferentially between liquid and vapour phases is the equilibrium ratio K_i . For a multi-component mixture, the vapour–liquid equilibrium data are represented in terms of *K*-values (vapour–liquid distribution ratios) defined by:

$$K_i = y_i / x_i \tag{11}$$

Where y_i and x_i are the mole fractions of component ‘i’ in the vapour and liquid phases

respectively. The values of the ratio K_i are correlated empirically or theoretically in terms of temperature, pressure and phase compositions.

In large-scale industrial distillation it is seen that *K* values are widely used in the design calculations of continuous distillation columns for distilling multicomponent mixtures. It is seen from the plot, that the *K*-value of only light hydrocarbons are considered.

We can observe that the vapour-liquid distribution ratio is high in the upper section of the fractionator column and then the values decline down the column and negligible for the last few trays of the fractionator column.

This plot is more important for the production of LPG. Since we are dealing with the estimation of gasoline production, we will neglect that plot.

(5) Light Liquid v/s Tray Position:

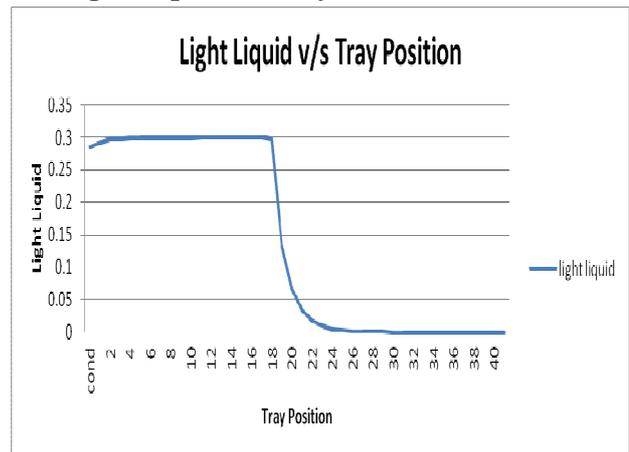


Figure 7: Plot of Light Liquids v/s Tray position

The primary end-products produced in petroleum refining may be grouped into four categories: light distillates, middle distillates, heavy distillates and others. The light distillates consist of Liquid petroleum gas (LPG), Gasoline (also known as petrol), kerosene, jet fuel and other aircraft fuel. Naphtha normally refers to a number of flammable liquid mixtures of hydrocarbons, i.e. a component of natural gas condensate or a distillation product from petroleum, coal tar, or peat boiling in a certain range and containing certain hydrocarbons. It is a broad term covering among the lightest and most volatile fractions of the liquid hydrocarbons in petroleum. In petroleum engineering, full range naphtha is defined as the

fraction of hydrocarbons in petroleum boiling between 30 °C and 200 °C.

It consists of a complex mixture of hydrocarbon molecules generally having between 5 and 12 carbon atoms. It typically constitutes 15–30% of crude oil, by weight. Light naphtha is the fraction boiling between 30 °C and 90 °C and consists of molecules with 5–6 carbon atoms. Heavy naphtha boils between 90 °C and 200 °C and consists of molecules with 6–12 carbons.

As it is seen in the plot, in Figure 7, most of the light liquids can be obtained from the initial trays of the fractionator column. In these initial trays, the light gases are obtained and with the help of further separation processes we hence obtain LPG and gasoline. Therefore it is beneficial that light liquids should be more at the top of the column as the light components are separated from the top of the fractionator column. In the middle section of the fractionator column, still consists of some light liquids.

It is from one of these trays only from where we draw off the light liquid and name it as light cycle oil (LCO). After tray number 18, we see that there is a sudden decline in the amount of light liquid in the bottom trays of the fractionator column. We find very negligible amount of light liquids as we proceed downwards in the column. That is because in the lower section of the column we draw off the heavy cuts and receive the residue at the bottom of the fractionator column.

(6) Transport Properties v/s Tray Position:

The transport properties (viscosity, thermal conductivity, etc) of fluids are important for the most efficient engineering design of many processes in the oil and chemical industries. They characterize the response of a fluid to changes in its temperature, speed of flow and/ or composition. Transport processes are the process whereby mass, energy or momentum is transported from one region of a material to another, under the influence of composition, temperature or velocity gradients. There are a large number of transport properties in principle, but three have, by far, the greatest practical and

scientific importance. They are diffusion coefficient, thermal conductivity and the viscosity and are associated with the transport of mass, energy and momentum respectively.

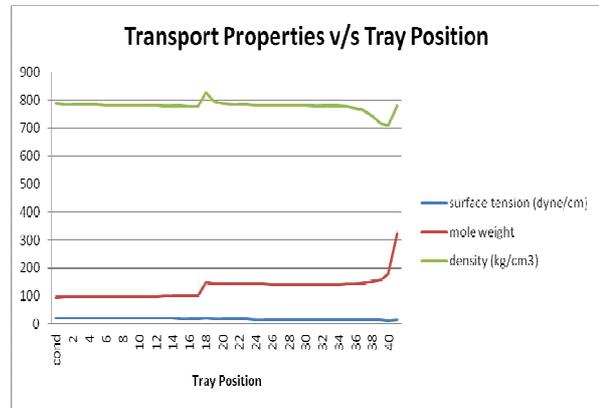


Figure 8: Plot of Transport Properties v/s Tray position (Part 1)

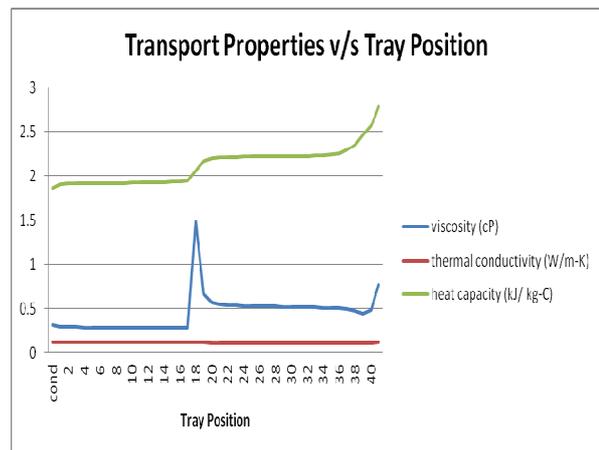


Figure 9: Plot of Transport Properties v/s Tray position (Part 2).

The transport properties discussed for the plots are density, mole weight, surface tension, heat capacity, viscosity and thermal conductivity. Properties like thermal conductivity and surface tension show no changes throughout the fractionator column, from top to bottom. On the other hand, the rest of the properties show a peculiar pattern in their behavior in the fractionator column. The other properties are initially steady at the top section of the column and then they change for the bottom section of the column. These changes occur at the tray number 18, exactly from the same tray number after which the light liquid rate reduce and only heavy liquid is obtained thereafter. Though the changes in these properties are not so drastic that

they could not affect the behavior of the fluid within the fractionator column, which hence could not affect the outlet streams.

The change in most of the plots is that the changes in the plotting are almost after the 18th tray, the tray after which the heavy liquids start to rule the fractionator column. Above 18th tray, mostly we find light liquid and light gases. From the light gases, we obtain LPG and gasoline with the help of further processes.

Since we are more concerned with the gasoline, hence for maximizing the production of it, we must have more flow rate of light liquids and vapours along with less of methane, ethane, propane and butane altogether in the upper section of the fractionator column.

[VI] CONCLUSION:

A model for preheater, riser, stripper, reactor and fractionator of modern UOP type FCC unit was developed. The proposed model is capable of predicting overall conversion, product yields, temperature and pressure. The model results are in close agreement with the industrial data and the data predicted by the simulator. The predictions of the FCC model are dependent on the value of cracking reactions rate constants, which can easily be obtained with the help of proposed model for different characteristics of the feed stocks, type of catalyst, activity of catalyst and operating parameters. Therefore, it seems to be more appropriate to use these rate constant parameters obtained for a pair of feedstock and catalyst.

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