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MODELING, SIMULATION AND OPTIMIZATION OF FCC DOWNER REACTOR

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Abstract

Downer reactor, in which gas and solids move downward co-currently, has unique features such as it accommodates high-severity operation at the initial stage with the benefit of near plug flow reactor. Literature have shown the downer could have advantages over riser. The purpose of downer reactor is to reduce the contact time to reduce the thermal cracking and eliminate back mixing to reduce dry gas formation and narrow the contact time distribution. In the present paper, mathematical model for downer reactor have been developed, in which a five-lump model is used to characterize the feed and the products, where gas oil crack to give lighter fractions and coke. There are present nine kinetic parameters and one catalyst deactivation activity. The integrated reactor steady state model makes gross assumption about the hydrodynamics, using Runga Kutta method. Optimization study of FCCU downer reactor to maximize its profitability and satisfy real-life constraints Non dominated sorting genetic algorithm (NSGA-II) is used, which is used to solve a two objective function optimization problem in this paper. The objective functions used are maximization of the gasoline yield, minimization of the catalyst flow rate. The optimal results obtained here provide physical insights that can help one in obtaining and interpreting such solutions.

Keywords: Fluid catalytic cracking; HS-FCC; FCC downer; Evolutionary algorithm; Non-dominated Sorting Genetic Algorithm(NSGA-II).

1. Introduction

The FCC unit plays a very important role in an oil refinery, because it converts heavy fractions (vacuum distillates or some vacuum resids) to gasoline, C_3-C_4 cuts and petrochemicals. The objective of fluid catalytic cracking process is to convert high molecular weight hydrocarbons (e.g. gas oil) coming from primary reefing, to more valuable lower weight hydrocarbon products in a safe, cost effective manner. Typical FCC units are composed of two reactors riser and regenerator the cracking reactor where almost all the endothermic cracking reactions and coke deposition on the catalyst occur; and the regeneration reactor, where air is used to burn off the coke on the catalyst. The catalyst that loses its activity in the reactor due to coke deposition is reactivated in the regenerator by burning off the coke utilizing air. The catalyst serves the purpose of catalyzing the reactants and supplying the necessary heat to the reaction [15]. The riser is a very efficient catalytic cracker; therefore all FCC units were upgraded to operate with a riser reactor. In the last three decades, some drawbacks of riser appeared. Thereafter many researches tried to analyze the main problems of the risers. The major disadvantage they documented was back mixing of catalyst particles inside the riser. Actually, a significant amount of catalyst is not used properly because of the back mixing phenomenon [7]. The high severity operation (e.g., high temperature or high solids flow rate) of risers, however, may cause enhanced coke and dry gas formation, especially limiting conversion and selectivity to liquid products, e.g., gasoline. As an alternative, the special features of this new process include a down-flow reactor which was proposed in the 1980s to achieve the desired reactor features [1].

1.1 High-Severity FCC Process

High-Severity Fluid catalytic cracking (HS-FCC) is a new process for the conversion of heavy oils into lighter hydrocarbon products and petrochemical feed stocks. Research teams from Japan and Saudi Arabia are jointly developing this technology. The process combines mechanical modifications to conventional FCC with changes in process variables and catalyst formulations. The main operating regime of the process is a special down-flow reactor system, high reaction temperature, short contact time, and high catalyst/oil ratio. The HS-FCC project shared between KFUPM petroleum energy Centre – Japan (PEC) aims to construct a pilot plant as shown in fig.1., which will give valuable information to prove whether the downer is better than the riser or not. Moreover, Nippon Oil Company , Japan, is also installing a cold model as demonstration unit for FCC downer process in Japan.

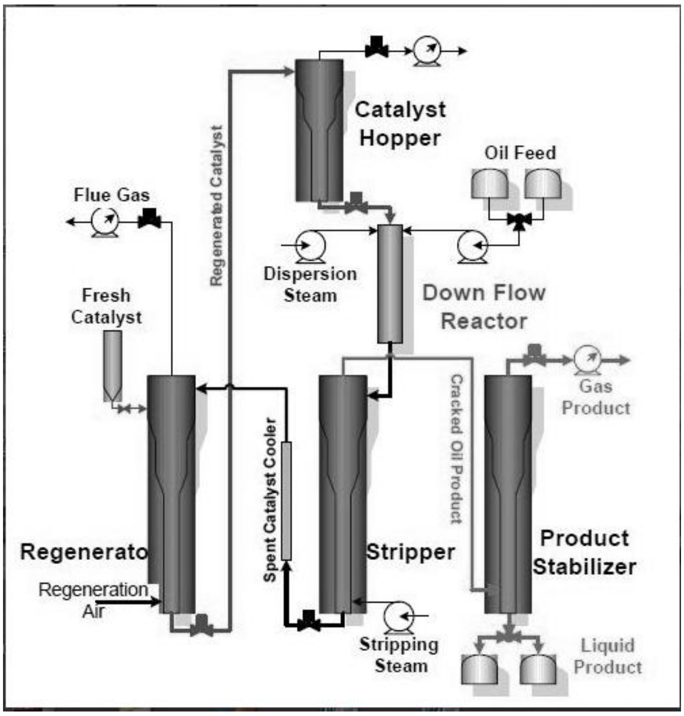

Fig.1 High-Severity FCC Process [8]

1.2 Downer reactor

A typical downer reactor consists of a vertical column (usually of circular cross-section, but sometimes square or rectangular) with gas and solids distributors at the top and one or more gas-solids separator at the bottom. For catalytic reactions, or gas phase reactions with solids as heat carriers, solids are recirculated to the top of the downer after regeneration or re-heating. In this new reactor gas and solids move vertically downward in the direction of gravity, the radial gas and solids flow structures are much more uniform compared to other gas–solids fluidized bed reactors, e.g., bubbling bed, turbulent bed and riser. Recent studies about downer reactors showed that almost plug flow of the solids can be achieved with FCC particles. However, the radial solids distribution still shows higher solids concentrations in the wall region compared to the core region [13,15,16]. Downer is therefore acknowledged as a novel multiphase flow reactor with great potential in high-severity operated processes, such as the high temperature, ultra-short contact time reactions with the intermediates as the desired products.

2. MODEL DEVELOPMENT

The HS- FCC process is similar to the conventional FCC. It consists of three components, a downer reactor, a catalyst stripper and a regenerator. In this model, the stripper role is not considered because it does not change the heat or the mass of the spent catalyst stripped from the product of the downer reactor. This unit deals with two reactors. First the downer reactor where the gasoil and catalyst are fed from the top of the downer causing the endothermic cracking reactions to occur.

2.1 DOWNER KINETICS

For the modeling of the downer reactor many schemes are proposed. Here [4] five lump scheme has been considered for present study. The below fig.2 represent the schematic diagram of the five –lump model.

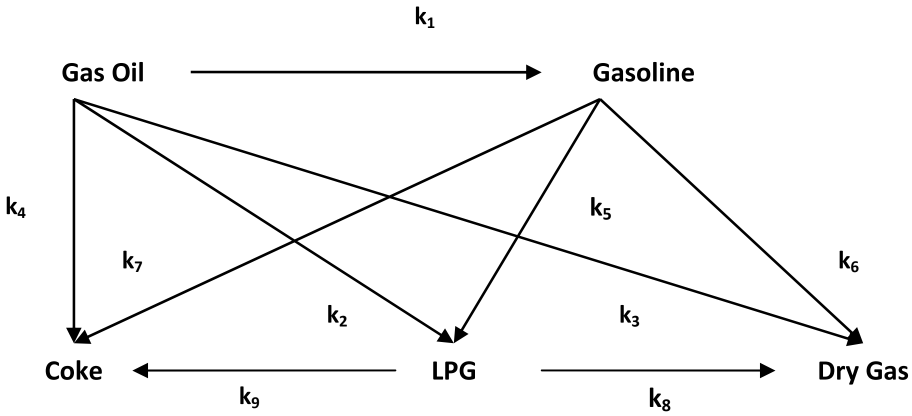

Fig. 2 Schematic diagram of the five-lump

For each reaction, a kinetic expression (ri) was formulated as a function of product yield (yi), deactivation function (φ) and kinetic constants (ki). Gas oil cracking was considered as a second order reaction and gasoline and LPG as first order [2]. The use of first order reaction for cracking of LPG has been discussed in the literature [9]. The exponential law was assumed for catalyst decay (φ). Based on these assumptions, the reaction rates for the five lumps are as follows:

$$GASOIL\,(r_1) = -(k_1 + k_2 + k_3 + k_4)(1-\varepsilon)y_1^2 \quad (1)$$

$$GASOLINE\,(r_2) = (k_1 y_1^2 - k_5 y_2 - k_6 y_2 - k_7 y_2)(1-\varepsilon) \quad (2)$$

$$LPG\,(r_3) = (k_2 y_1^2 + k_5 y_2 - k_8 y_3 - k_9 y_3)(1-\varepsilon) \quad (3)$$

$$DRYGAS\,(r_4) = (k_3 y_1^2 + k_6 y_2 + k_8 y_3)(1-\varepsilon) \quad (4)$$

$$COKE\,(r_5) = (k_4 y_1^2 + k_7 y_2 + k_9 y_3)(1-\varepsilon) \quad (5)$$

2.2 DOWNER REACTOR MODELLING

1. Both catalyst and feed oil is charged in to the upper part of the downer reactor. Instantaneous vaporization of feed oil occurs by taking latent heat and sensible heat from the hot catalyst. Thus feed oil and catalyst are in thermal equilibrium.
2. There is no loss of heat from the downer and the temperature of the reaction mixture (vapor +catalyst) falls only because of endothermicity of cracking reaction.
3. Plug flow behavior is assumed for the downer according to the survey of hydrodynamics studies.
4. The changes due to molar expansion were not accounted. Thus the molar volume of hydrocarbons is constant along the downer. This assumption simplifies the derivations of the equation by justifiable idea as proved by [12].
5. The role of steam used to disperse the feed at the entrance of downer is neglected due to its low amount compared with the feed. Its percentage in the fed is about 2%.

6. Vapor phase and solid mass flow rate are constant and independent of position. Likewise, the gases void fraction is assumed constant and independent of position.
7. The downer has high combined stream velocity and very short residence time. Thus, it can be assumed that the dynamic term due to vapor phase concentration , coke formation and downer temperature in the regenerator. Therefore the mass and energy balance equations are considered at steady state.
8. Heat and mass transfer resistances are assumed as negligible.
9. There are no radial temperature gradient in gas & solid phase.
10. Catalyst deactivation follows the [14] which is non selection and related to coke on catalyst only.
11. Gas oil cracking is a second order reaction but cracking of gasoline and LPG are first order reaction.
12. Heat of reaction are assumed constant. Other thermal and physical properties are also assumed constant (heat capacities and densities) through the length of reactor.

On the basis of above discussion, the mole balance for the j^{th} lump over a differential element for downer reactor model can be written as follows :

$$\frac{dF_j}{dh} = -A_{dow} H_{dow}\, \rho_C \phi \sum_{i=1}^{9} \alpha_{ij}(-r_i) \quad j = 1, 2, ...5 \qquad (6)$$

Where j = 1 to 5 represents gas oil, gasoline, LPG, dry gas, and coke respectively. i = 1 to 9 represents the reactions as shown in Fig.2The rate equation in (kmol)/m3(s) are given by following ex expressions:

$$MW_g = \sum_{j=1}^{5} x_j MW_j \qquad (7)$$

$$r_i = k_{0,i} \exp(-\frac{E}{RT}) C_1{}^2 \phi(1-\varepsilon)\rho_c \quad \text{for i = 1,2,3,4} \qquad (8)$$

$$r_i = k_{0,i} \exp(-\frac{E}{RT}) C_2 \phi(1-\varepsilon)\rho_c \quad \text{for i = 5,6,7} \qquad (9)$$

$$r_i = k_{0,i} \exp(-\frac{E}{RT}) C_3 \phi(1-\varepsilon)\rho_c \quad \text{for i = 8,9} \qquad (10)$$

Where, C_1, C_2 and C_3 are concentration of gas oil, gasoline and LPG respectively. Other parameters can formulated as follows

$$\rho_V = \frac{P_{dow} MW_g}{RT} \qquad (11)$$

$$\alpha_{ij} = \frac{MW_i}{MW_j} \qquad (12)$$

2.3 Catalyst deactivation

Catalyst used for the cracking loses its activity mainly due to following three reason :

(i) Physical change due to coke deposition and structural change due to sintering.
(ii) Poisoning due to the presence of metals and non-metals in FCC feed.
(iii) Deposition of coke on the active site.

For the modeling of the catalyst deactivation the function ϕ was related to coke on catalyst as follows [14]:

$$\phi = (1 + 51C_c)^{-2.78} \qquad (13)$$

2.4 Energy balance around the downer reactor

The energy balance of plug flow reactor is applied for this model. Due to the endothermic cracking reactions in the downer, there is a temperature drop along the height of the downer. The enthalpy balance across a differential element of height dh of the downer can be represented as follows:

$$\frac{dT}{dh} = \frac{-A_{dow}H_{dow}}{F_{rgc}C_{P_C} + F_{feed}\sum_{i=1}^{5} x_i C_{P_{fvi}}} \sum_{i=1}^{9} r_i(\Delta H_i) \quad (14)$$

At the entrance of the downer:-The regenerated catalyst and preheated liquid are mix at the top of the reactor. So in order to define mix temperature it is necessary to write an enthalpy balance equation:-

$$T_M = \frac{F_{rgc}C_{P_c}T_{rgn} + F_{feed}C_{P_{fl}}T_{feed} + \Delta H_{evp}F_{feed}}{F_{rgc}C_{P_c} + F_{feed}C_{P_{fvgasoil}}} \quad (15)$$

Table 1. Kinetic and deactivation parameters for reaction in the downer and regenerator used in FCC unit (5-lump) [4]

Rate constant	Frequency factor	Activation energy (kJ/kmol)
k1	19584.55	57540
k2	3246.45	52500
k3	559.90	49560
k4	41.44	31920
k5	65.40	73500
k6	0.00	45360
k7	0.00	66780
k8	0.32	39900
k9	0.19	31500

Table 2. Heat of reaction and vaporization used in the FCC-downer reactor [4]

Heat of reaction	Value (kJ/kmol)
H1	45000
H2	159315
H3	159315
H4	159315
H5	42420

Table 3. Operational Parameters used to the FCC –downer reactor unit

Parameters	Value	Ref
Downer length (m)	5.8-11 m	From review
Downer diameter (m)	80mm-150mm	From review
Feed flow rate (kg/s)	0.4-1.2	[8]
Feed preheat temperature (K)	523 or 640	[8,17,18]
Regenerator temperature (K)	930.2	[4]
Catalyst flow rate (kg/s)	100-250	[8,17,18]
Downer pressure (atm)	0.079-1.25	[8,17,18]

Table 4. Physical and thermal properties used in the simulation of the FCC downer unit

Properties (unit)	value
$C_{P,c}$ (kJ/kg K)	1.108 kJ/ (kg K)
$C_{P,fl}$ (kJ/kg K)	2.10 kj/kg K
$C_{P,fv}$ (kJ/kg K)	2.04
ΔH_{evp} (kJ/kg)	270 kJ/ kg
X_{Pt}	0.10(x)
ρ_c (kg/m^3)	1500
C_H (kg H_2/kg coke)	12-30

3. Optimization

Optimization refers to finding the values of decision variables, which correspond to and provide the maximum or minimum of one or more desired objectives. optimization finds many applications in engineering, science, business, economics, etc. Without optimization of design and operations, manufacturing and engineering activities will not be as efficient as they are now. Several studies have also been carried out on the optimization of FCCUs. Most of them use some type of a profit-function as the objective. Some of the commonly used decision variables in these studies are the regenerator temperature, reactor temperature, catalyst circulation rate and the air supply rate. Here I am using recent adaptation of genetic algorithm (NSGA-II), as developed by Deb and co-workers [6] there are two versions of non- dominated sorting genetic algorithm NSGA [11] and the elitist NSGA-II [6]. These two adaptations of NSGA have been used extensively to solve a variety of multi-objective optimization problems in chemical engineering. The applications of NSGA (and other techniques) in chemical engineering have been reviewed by [3] while those of NSGA-II have been reviewed by [10], the latter for problems in chemical reaction engineering.

3.1General description of NSGA-II

(i) Population initialization

The population is initialized based on the problem range and constraints if any.

(ii) Non-Dominated sort

Once the population is initialized the population is sorted based on non-dominant set in the current population and the second front being dominated by the individuals in the first front only and the front goes so on.

(iii) Crowding distance

Once the non-dominated sort is complete, the crowding distance is assigned. Since the individuals are selected based on rank and crowding distance, all the individuals in the population are assigned a crowding distance value. Crowding distance is assigned front wise and comparing the crowding distance between two different fronts is meaningless.

(iv) Selection

Once the individuals are sorted based on non-domination and with crowding distance assigned, the selection is carried out using a crowded-comparison-operator (n).

(v) Recombination and selection

The offspring population is combined with the current generation population and selection is performed to set the individuals of the next generation. Since all the previous and current best individuals are added in the population, elitism is ensured. Population is now sorted based on non-domination. The new generation is filled by each front subsequently until the population size exceeds the current population size. If by adding all the individuals in front Fj the population exceeds N then individuals in front Fi are selected based on their crowding distance in the descending order until the population size is N. And hence the process repeats to generate the subsequent generations.

4. RESULT AND DISSCUSION

This section discusses the results obtained by simulation and optimization of FCCU downer. This section is organized into two parts:

1. Optimization of FCCU downer reactor.
2. Simulation of model equations for a downer reactor.

4.1 Optimization of FCCU downer reactor

Following Figures show the plot between the two objective functions:

(i) Maximization of gasoline yield

(ii) Minimization of catalyst flow rate

The population size was 100 and the max. number of generation was taken as 200 (min. zero and max. 200).the computer time was about 72 hr. It can be observed from figures that every point on the pareto surface is non dominating because any point may be good than other in terms of two objective function.

Table 5. Parameters and bounds used in optimization

Parameter	Value
Population size	100
Probability of crossover	0.95
Probability of mutation	0.05
Rand state	0
Maximum generation	200

Bounds:
575 K < Feed preheat temperature < 640 K;
126 kg/sec < Catalyst flow rate in first reactor < 315 kg/sec;
0.38 kmole/sec < Air flow rate <0.78 kmole/sec,
150 K< Air preheat temperature <425 K.

Fig.3 shows plots of gasoline yield and random populations of decision variables (catalyst flow rate) in downer reactor at zero generation which were generated using the Rand command in MATLAB^{TM}. Fig.4 shows the plot of gasoline yield and decision variables (catalyst flow rate) in downer reactor at 200 generation.

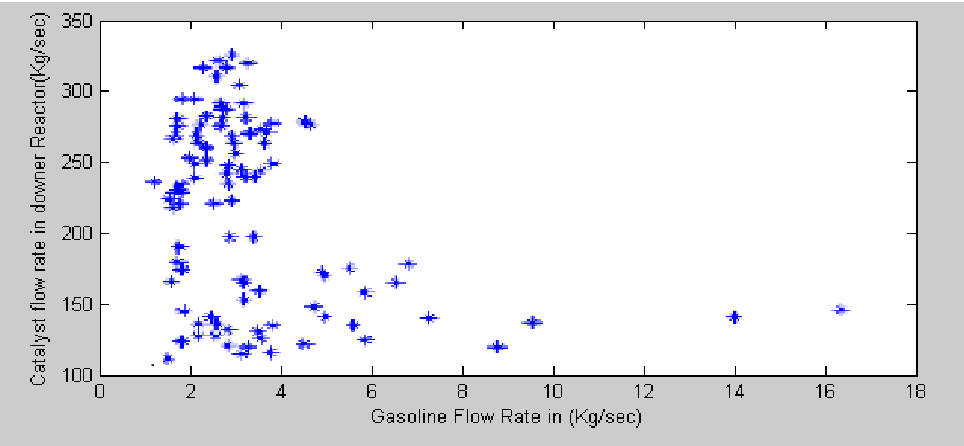

Fig. 3. Population for zero Gen (Gasoline flow rate vs Catalyst flow rate in reactor

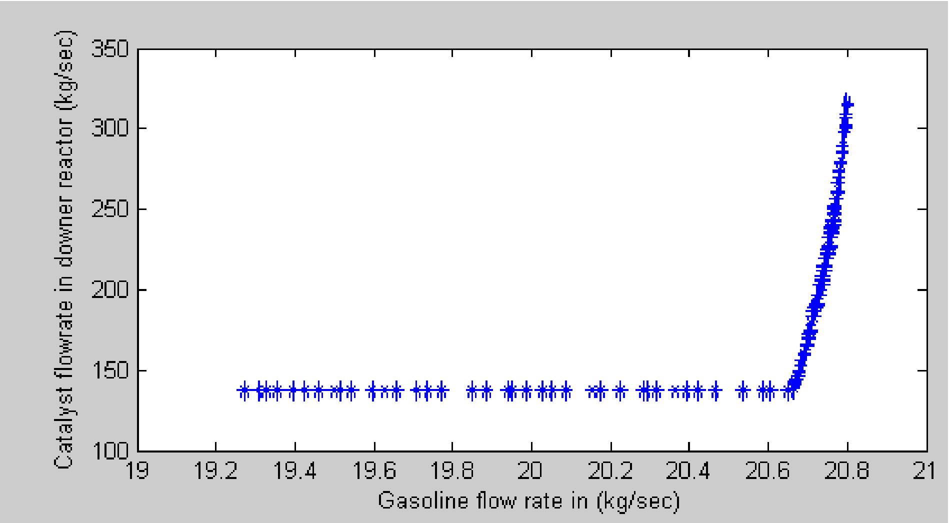

Fig. 4. Population for 200 Gen (gasoline flow rate vs catalyst flow rate in reactor

It can be easily inferred from Figure 4 that the catalyst flow rate in downer reactor should be always maintained close to the lower bound and it is also inferred that the gasoline yield constant up to some extant then it is slowly increases with increase in catalyst flow rate in reactor. Therefore, to minimize the catalyst flow rate we should maintain the catalyst flow rate close to the lower bound in reactor. From the optimized data it was also observed that feed preheat temperature and air flow rate should be maintained close to upper bounds and air preheat temperature should be maintained between 150 K and 425K.

4.2 Simulation of model equations for a downer reactor

Model equations for single stage riser developed by [4] were simulated. Fig.5 shows the formation of products from gasoil along the length of the downer. Fig.6 shows the temperature profile inside the downer. .

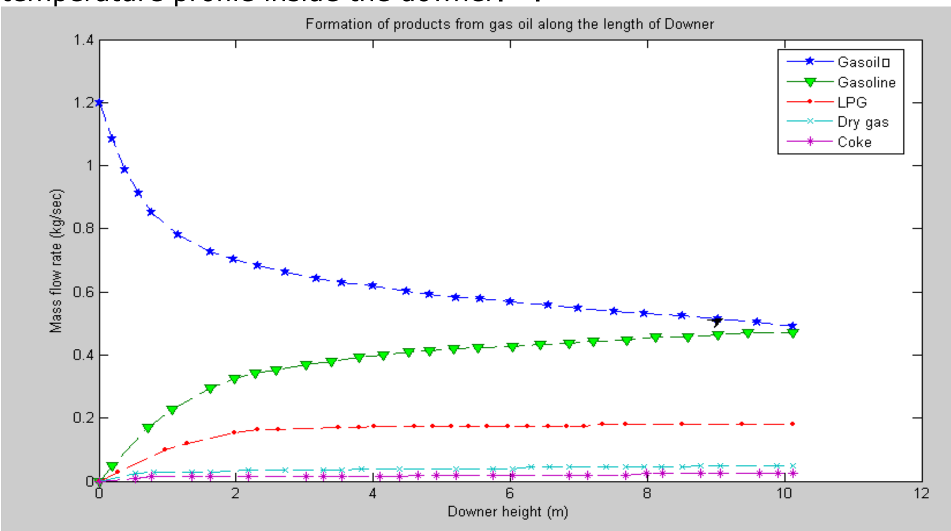

Fig. 5. Formation of products from gasoil along the length of downer

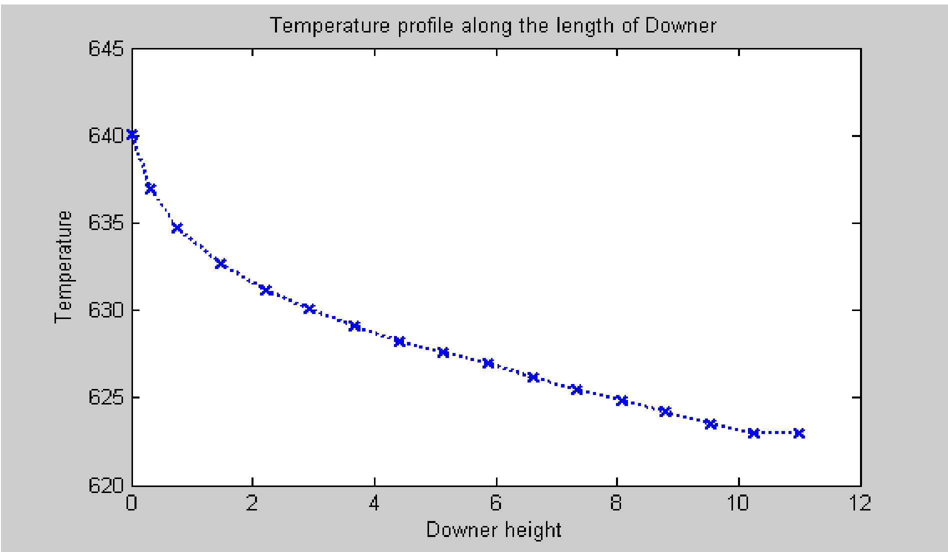

Fig. 6. Temperature profile along the length of downer

From table 5 it is observed that the gasoline yield 39.68 % for downer reactor and it was also observed that the temperature inside the downer and regenerator was more compared to that of single stage FCCU. It was also observed that this increase in gasoline yield was obtained at the cost of increased catalyst rate, increased feed preheat and the temperature of bottom of the reactor is 623 K . Remaining results are tabulated as follows:

Table 5. Simulation Results for downer reactor

Parameters	Results
Feed flow rate (kg/s)	1.2
Feed preheat temperature (K)	640
Catalyst flow rate (kg/s)	214.16
Downer pressure (atm.)	0.0950
Downer bottom temperature (K)	623.43
Gas oil (unconverted) (%)	40.16
Gasoline (%)	39.68
LPG (%)	13.76
Dry gas (%)	4.174
Coke (%)	2.226

5. Conclusion

In this work, we have presented model equations for an FCC downer-type unit. The results support the fact that in the downer, backmixing is eliminated and the overcracking of intermediate products is suppressed. At high severity conditions, a favorable shift in the product yields is obtained by downer; gasoline yield is increased, coke and dry gas yields are decreased. Though the light olefins yield is lower in case of downer, the total yield of useful products (gasoline+light olefins) is higher in downer as compared to the same from a riser. The increased yield of gasoline form downer can be converted to light olefins .

It was also observed that this increase in gasoline yield was obtained at the cost of increased catalyst rate, increased feed preheat and air preheat temperatures and increased regenerator pressure. Therefore, a cost analysis of operating cost and profit from production of excess gasoline is required.

Nomenclature

A_{dow}	cross-sectional area of downer, m^2
C_c	coke on catalyst at any location, (kg of coke) (kg of catalyst)$^{-1}$
C_i	concentration of i^{th} lump, kmol m^{-3}
C_{pc}	heat capacity of catalyst, kJ kg^{-1} K^{-1}
C_{pfl}	heat capacity of liquid feed, kJ kg^{-1} K^{-1}
C_{pfv}	heat capacity of vapor feed, kJ kg^{-1} K^{-1}
E_i	activation energy of i^{th} reaction, kJ $kmol^{-1}$
F_{rgc}	flow rate of regenerated catalyst, kg s^{-1}
F_{feed}	feed flow rate of oil, kg s^{-1}
F_j	molar flow rate of j^{th} lump, kmol s^{-1}
h	dimensionless height of downer
ΔH_{evp}	heat of vaporization of gas oil feed, kJ kg^{-1}
H_i	heat of formation of i, kJ $kmol^{-1}$
ΔH_i	heat of ith reaction, kJ $kmol^{-1}$
H_{dow}	height of downer, m
$k_{0,i}$	frequency factor for i^{th} reaction
k_i	reaction rate constant for i^{th} reaction
MW_c	molecular weight of coke, kg $kmol^{-1}$
MW_g	average molecular weight of gas phase, kg $kmol^{-1}$
MW_j	molecular weight of j^{th} lump, $j=1,2,\ldots,5$, kg $kmol^{-1}$
P_{dow}	pressure in , downer atm
r_i	rate of the i^{th} reaction, i=1-9 (riser);
R	universal gas constant, J K^{-1} $kmol^{-1}$
T_M	top temperature for heat balance calculations, K
T_{feed}	temperature of gas oil feed, K
T_{dow}	temperature of downer at any location, K
T_{rgn}	temperature (uniform) of dense bed, K
$T_{dow, bottom}$	temperature at bottom of downer, K
x_j	mole fraction of j^{th} lump, j= 1, 2, ..., 5
y_j	weight percent of hydrocarbons in the downer , where j=1,2,3…..

Greek Letters

α_{ij} stoichiometric coefficient of j^{th} species in ith reaction, based on mass
ε void fraction in downer at any location
ρ_c density of solid catalyst (not including void fraction), kg m^{-3}
ρ_v density of vapor at any location, kg m^{-3}
φ activity of the catalyst

Subscripts

i, j i^{th} or j^{th} lump (1, gas oil; 2, gasoline; 3, LPG; 4, dry gas; 5, coke)

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