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Simulation of Fcc Riser Reactor using Five Lump Model

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Abstract : Five-lump kinetic model has been studied to predict the conversion of feed oil and formation of gasoline and coke with different space time at different temperature and different catalyst to oil ratio. The developed model has been studied using C++ programming language using Runge-Kutta Fehlberg mathematical method. The five-lump model is capable of predicting the deposition of coke on the catalyst and yield of LPG, light gases gasoline. By the use of five-lump model, 91% conversion of feed oil and 47 mass% gasoline yield was obtained at 595K in 7.2 s space time. In addition to this, effects of space time and temperature on the yield of coke gasoline and conversion of gas oil have been presented. Effect of, catalyst to oil ratio is also considered in studies.

Key Words : Fluid catalytic cracking Riser, Five-lump model, Gas-oil, LPG.

Introduction

Fluid Catalytic Cracking[1] is considered to be one of the most important processes in the petroleum refinery industry. It is the heart of modern refinery. It is the process in which heavier hydrocarbon molecules are converted to lighter molecules which are useful products like gasoline, LPG etc. The hydrocarbon feed enters a transport bed tubular reactor (riser) through feed atomizing nozzles and comes in contact with the hot catalyst coming from the regenerator. The feed gets vaporized and cracks down to the lighter molecules as it travels upwards along with the catalyst. As a result of cracking, the velocity of the vapors increases along the riser height.

Coke, which is the byproduct of cracking reactions, gets deposited on the catalyst surface thus causing the catalyst to lose its activity. The cracked hydrocarbon vapors are separated from the deactivated catalyst in a separator. The vapors adsorbed onto the surface of the catalyst are also stripped off using steam in the catalyst stripper. The cracked hydrocarbon vapors are sent to the main distillation column for further separation into various fractions, and the deactivated catalyst flows into the regenerator. In the regenerator, the coke deposited on the catalyst surface is burned off to regenerate the catalyst. The catalyst also becomes hot during the regeneration process. This hot-regenerated catalyst is recycled back to the riser reactor. Thus the catalyst acts as a heat carrier also and provides the heat required for endothermic cracking reactions in the riser reactor as well as the heat required for the vaporization of feed.

A three lump model[2] have been developed for the cracking reactions taking place in the riser reactor. The three lump model consists of one a feedstock lump (gas oil, Volatile Gas Oil (VGO) or any other heavy feed) and two product lumps: a) gasoline b) coke and light gases. The gasoline lump contains the fraction between C_5 up to the hydrocarbons with boiling temperature around 220°C. The coke and light gases lump contains in addition to coke, C_4 and lighter than C_4 hydrocarbons.

Next, the coke was separated out of the light gas, considering it as two separate lumps C_1-C_4 gas and coke, thus developed the first four lump model[3,4] for FCC.

The four lump model was extended to five lumps[5]. The authors further divided the gases lump into two different lumps: a) dry gas, b) liquefied petroleum gas (LPG). LPG can be formed either directly from gas oil or as a secondary product from gasoline over cracking. On the other hand, dry gas (H_2, C_1, C_2) can be formed either directly from gas oil cracking or as a secondary product from gasoline and LPG cracking.

2. Process Description

The FCC unit consists of two reactors, (1) The riser reactor, where almost all the endothermic cracking reactions take place and also coke deposition on the catalyst occur, (2) The regenerator reactor, where air is used to burn off the coke. The regeneration process, in addition to reactivating the catalyst pellets, provides the heat required by the endothermic cracking reactions.

Figure 1 shows a typical FCC process[6] that consists of two major operating parts, the reactor riser and the regenerator. The cracking of the hydrocarbon feed takes place in the riser, while the regenerator does the work of reactivating the catalyst by burning the coke deposited on the catalyst in the riser reactor. The feed is then preheated to a temperature of 450-600 K in a furnace or in a pump-around from the main-fractionator.

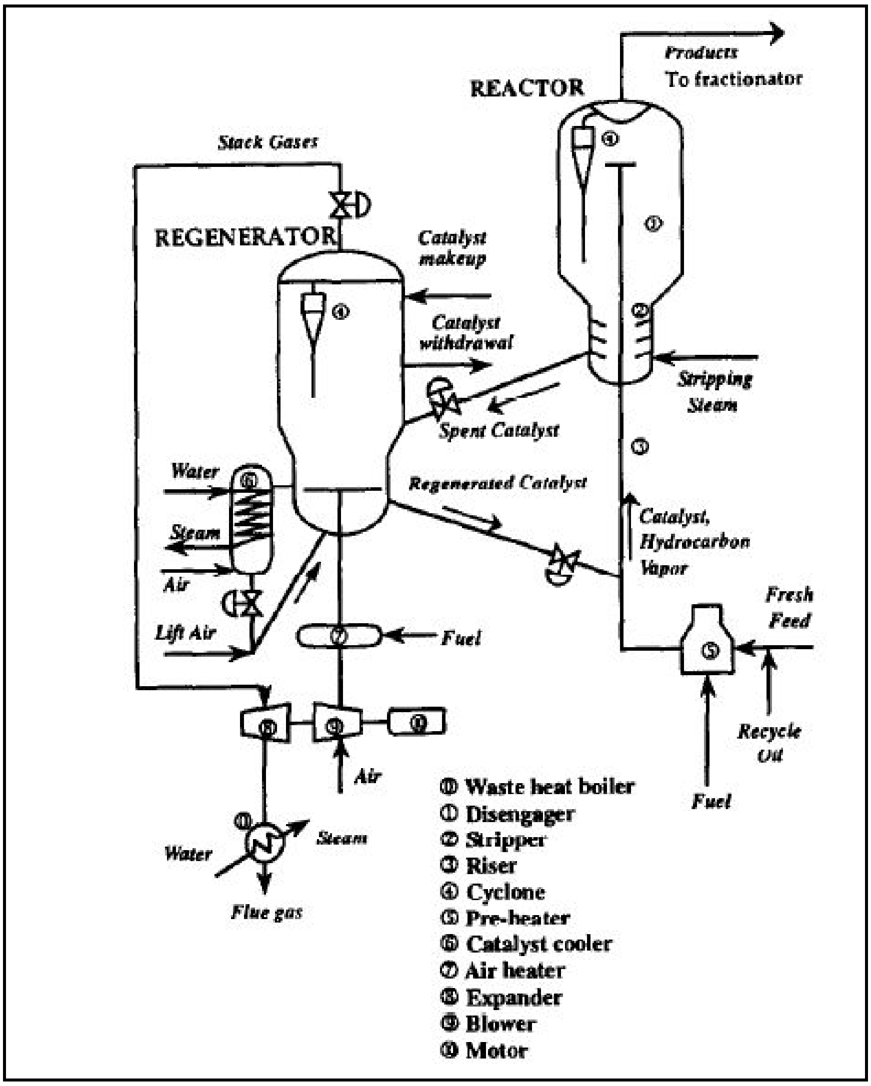

Figure 1: Schematic diagram of fluid catalytic cracking unit

The hydrocarbon vapors undergo endothermic catalytic cracking reactions as they move up through the riser reactor. Lighter hydrocarbons are produced as main cracking products along with by-product coke which deposits on the catalyst surface and this also lowers the catalyst activity.

3. Five-Lump Model:

An improved and updated model[7] for modern fluidized bed catalytic cracker (FCC) has been presented. A five lump model is proposed to describe the process as shown in figure 2. The riser bed acts as a transported bed, with combined stream velocity and a short residence time in the order of a few seconds.

Thus it can be assumed that the dynamics of the riser in comparison with the coke burning and temperature changes in the dense phase of the regenerator are negligible. Therefore the mass and energy balance equations in the riser are considered at quasi steady state[8,9]. This model is different from other mainly in that the deposition rate of coke on catalyst can be predicted from the gas oil conversion and isolated from light gas yield. Also LPG (Liquefied Petroleum Gas) i.e., the C_3-C_4 is considered a separate lump and the composition can be individually explained. A five-lump model is thus proposed for the reactor kinetics to examine coke formation with conversion yield of gasoline.

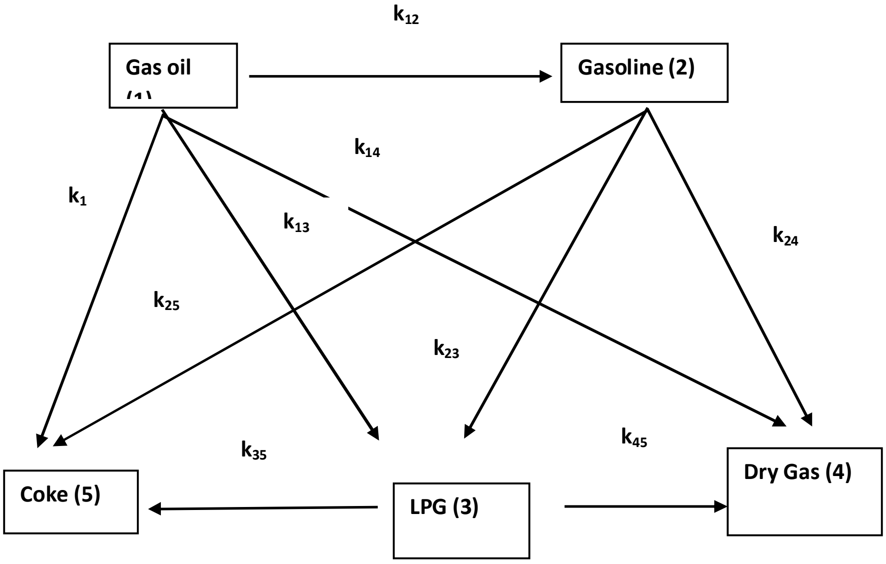

Figure 2: Five-Lump Kinetic Model

In order to develop kinetic model following assumptions were made:

- There is no interaction between coke and C_1-C_4 gas
- Gas flow in the reactor is in ideal plug flow
- Axial dispersion in the reactor is considered to be negligible
- Gas-oil cracking reaction is second order reaction
- Gasoline cracking reaction is first order reaction
- Both gas oil and gasoline have identical activity decay function φ
- Light gas does not produce coke, which is mainly produced from aromatic hydrocarbons
- Coke intent in feed is very low
- The riser wall is adiabatic
- Feed viscosity and heat capacities of all components are constant
- Adsorption and dispersion inside the catalysts particles are negligible
- Pressure changes throughout the riser-height are due to static head of catalyst in the riser

The second order reaction can be attributed to the wide range of crack ability of the molecules in the feed lump thus, some components in the feed crack very readily, while others are more refractory to cracking. As the reaction proceeds, the more readily cracked components crack first, with the reaction appearing to slow down as the more refractory materials now dominate with their lower rate. Rate constants decay rapidly as coke is laid down on catalyst, it is necessary to integrate catalyst decay with the kinetics.

Gas Oil

$$\frac{dy_1}{dt_v} = (-k_{12} - k_{13} - k_{14} - k_{15})\, y_1^2 \phi$$

Gasoline

$$\frac{dy_2}{dt_v} = (k_{12}\, y_1^2 Ø - k_{23}\, y_2 Ø - k_{24}\, y_2 Ø - k_{25}\, y_2 Ø)\ \text{LPG}$$

$$\frac{dy_3}{dt_v} = (k_{13}\, y_1^2 Ø + k_{23}\, y_2 Ø - k_{34}\, y_3 Ø - k_{35}\, y_2 Ø)\ \text{Fuel Gas}$$

$$\frac{dy_4}{dt_v} = (k_{14}\, y_1^2 Ø + k_{24}\, y_2 Ø + k_{34}\, y_3 Ø)$$

Coke

$$\frac{dy_5}{dt_v} = (k_{15}\, y_1^2 Ø + k_{25}\, y_2 Ø + k_{35}\, y_3 Ø)\quad Ø=\exp(-\alpha t/c)$$

Based on the above assumptions and from the five-lump model diagram, the overall reaction can be expressed in equations as shown above, in addition, the energy for five lump model is given below:

$$\frac{dT_{ref}}{dt_v} = -F_{tf}/(F_{gc}C_{p,c} + F_{tf}C_{p,fv})\, Ø\ [\, y_1^2(k_{12}\Delta H_{12} + k_{13}\Delta H_{13} + k_{14}\Delta H_{14} + k_{15}\Delta H_{15}) + y_2(k_{23}\Delta H_{23} + k_{24}\Delta H_{24} + k_{25}\Delta H_{25}) + y_3(k_{34}\Delta H_{34} + k_{35}\Delta H_{35}) + H_{Iris}$$

The boundary conditions at $t_v = 0$;

$y_1(0) = 1$
$y_2(0) = 0$
$y_3(0) = 0$
$y_4(0) = 0$
$y_5(0) = 0$

If the catalyst assumed to be in plug flow, the differential equations can be solved for the system variables. The kinetics of the FCC reactor depends on the process variables and parameters such as temperature, space time, ratio of catalyst circulation rate to oil mass flow rate, regenerator temperature, gas oil pre heat temperature, physical properties of the gas oil and catalyst. Usually, feed and catalyst conditions do not change frequently. Thus, they are not considered as process variables. The models at steady state are solved by the Runge-Kutta-Fehlberg method by using the kinetic parameters are given in the table 1.

Table 1. Five-lump kinetic data[7]

Rate Constant	**Frequency Factor**	**Activation Energy (kJ/kmol)**	**Heat of reaction (kJ/kmol)**
k_{12}	18579.9	57540	45000
k_{13}	3061.1	52500	159315
k_{14}	532.14	49560	159315
k_{15}	39.04	31920	159315
k_{23}	65.4	73500	42420
k_{24}	0.00	45360	42420
k_{25}	0.00	66780	42420
k_{34}	0.32	39900	2100
k_{35}	0.19	31500	2100

Table 2.1 Feed Properties and Conditions

Feed Properties and Conditions	
API	24.70
K_{UGP}	12.19
Inlet feed temperature	609K
Feed	Gas Oil
Specific Heat	3.430 kJ/kg/K

Table 2.2 Process Conditions of the Riser-Reactor

Riser-Reactor	
Gas oil flow rate	55.56 kg/s
Regenerated catalyst flow	308.5 kg/s
Catalyst to oil ratio	5.55
Riser Temperature	595K-755K
Gas oil residence time	2-10s
Pressure	2.6-2.8 kg/cm^2
Stripping steam	0.718kg/s
Make-up catalyst flow	0.417 kg/s
Nozzles	4
Inclination of nozzles	90^0

Table 2.3 Process Conditions of the Regenerator

Regenerator	
Regenerated catalyst temperature	945 K
Flue gas temperature	978 K
Regenerator temperature	1000-1200 K
Pressure	3.10 kg/cm^2
Entrained catalyst flow rate	0.023 kg/s

4. Results

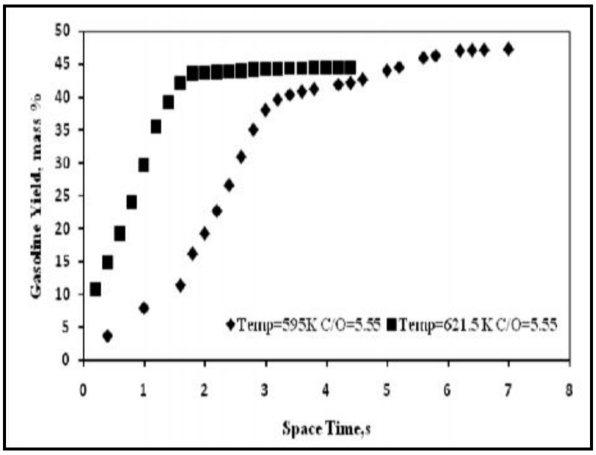

Figure 3a: Gasoline yield as a function of space time.

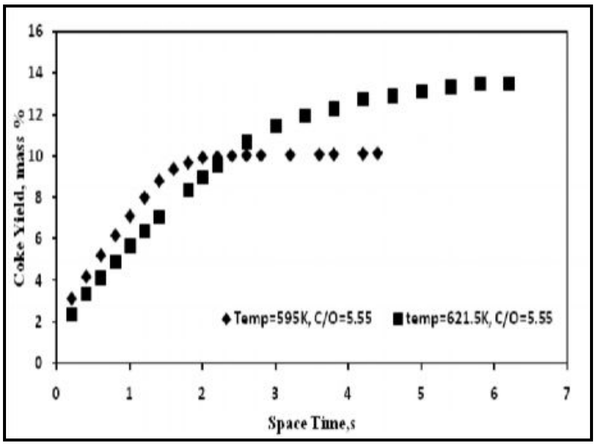

Figure 3b: Coke yield as a function of space time

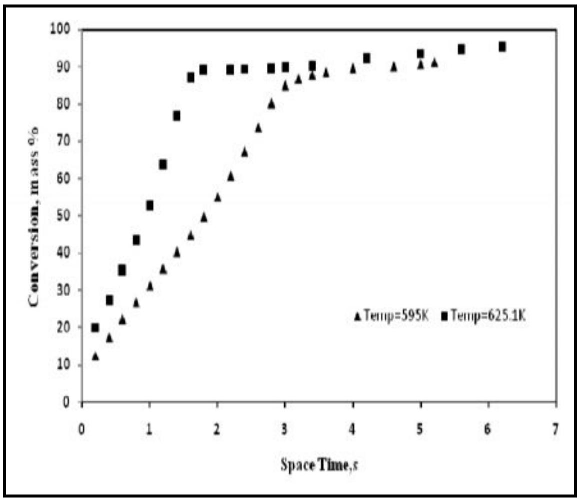

Figure 4a: Effect of space time on gas oil conversion

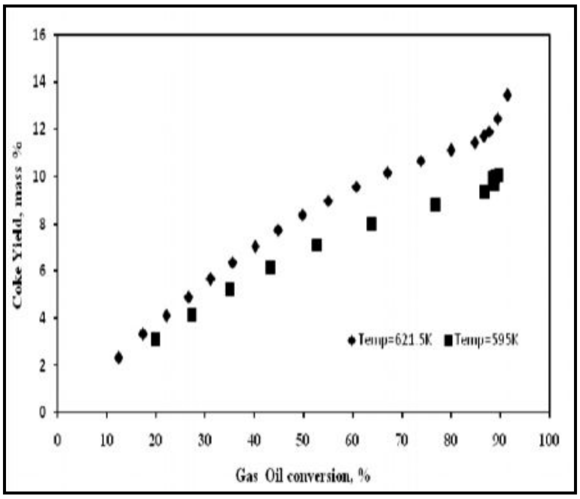

Figure 4b: Coke yield as a function of gas oil conversion at different temperatures

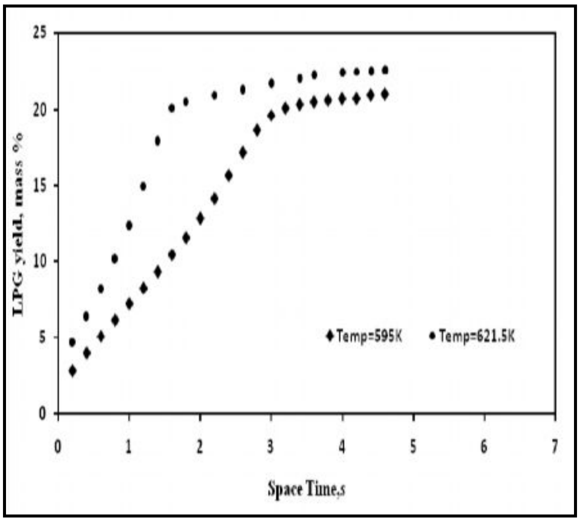

Figure 5: LPG yield as a function of gas oil conversion at different temperatures

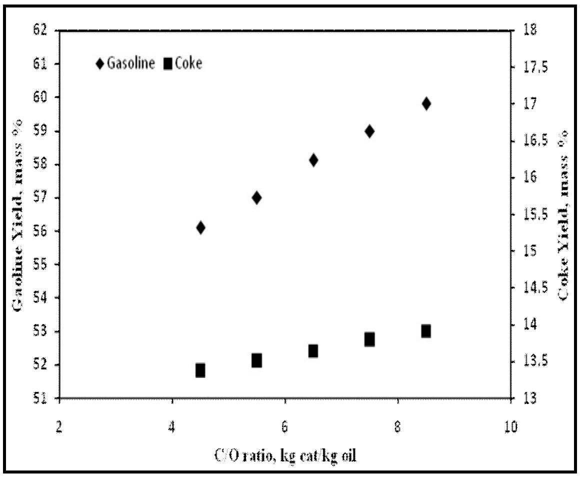

Figure 6 Effect of C/O ratio on yield of various products

5. Discussions

Effect of space time and temperature:

Results of simulation run are plotted in figure 3a. It is seen that as space time increases gasoline yield increases. The gasoline yield is around 44 and 45 mass % at a temperature of 595 K and 621.5 K respectively in space time of 4.2 s. The yield is increased to 48.6% in 7.2s at 595 K. Coke yield is noted to be 10 mass % and 13 mass % at 595 K and 621.5 K respectively. Effect of space time is presented in figure 4. Figure 4a shows conversion increased with increase in space time up to value of 6.5 s. At temperature 595 K, maximum 85 mass% conversion is seen in space time 3 s, which reached to 95 mass % in 5.5 s. The LPG yield at a space time of 5 s, at 621.5K is 23% and 21% at 595 K (figure 4b). Yield does not increase much with space time. These data show 2 s and 3 s are reasonable space time at temperature 621.5 K and 595 K respectively. At higher temperature a higher volume of gas oil is cracked in a lesser space time. It is concluded that although the gas oil conversion at higher temperature is more, but the yield of gasoline is lower. It is observed that at 621.5 K, the riser reactor converts a greater amount of gas oil in the figure 4a and also the production of light gases also increases and gasoline yield decreases. If the length of the riser reactor is increased or space velocity is lowered for further conversion, then the gasoline starts decomposing and forms secondary products. Effect of temperature with increase in gas oil conversion for coke formation is presented in figure 5. When gas oil conversion increases to 90%, the coke yield increases to 13 mass % at 621.5 K and 11 mass % at 595 K. More coke is formed with more conversion of gas oil.

Effect of catalyst to oil ratio:

C/O ratio is an important factor as it is relates to the number of active sites available for gas oil cracking. It is a primary variable, controlled by changing the catalyst circulation rate. The study is conducted by varying the C/O ratio between 4-10. Increase in C/O ratio increases the conversion as well as the reactor temperature. Since cracking reactions are endothermic, increase in temperature is moderated by additional cracking, which is due to increased catalyst circulation rate. Recycled catalyst has a higher temperature than the riser reactor as it comes from the regenerator. As shown in figure 5a, when the C/O ratio is 4.5 the gasoline yield is 55.89%. However as the C/O ratio is increased the gasoline yield starts increasing, yield of 58.9% at a C/O ratio of 8.5 is obtained. Coke formation is also increased, which has a value of 13.3%-14%.

6. Conclusions

The differential equations formed by the catalytic cracking reactions have been simulated. The model presented in the literature is solved at steady state condition using the Runge-Kutta-Fehlberg method for a set of ordinary differential equations. The code language used is C++ language. The simulation results are found to be in the right trend.

The increase in temperature leads to the rise in conversion of gas oil. However there is also an increase in yield of coke. Hence a significant optimum temperature is required to be maintain throughout the riser reactor.

Space time is another important factor in simulation of riser reactor. An increase in space velocity will cause gas oil conversion to increase as the contact between gas oil and catalyst is more. A lower space velocity will favor yield of gasoline.

The increase in catalyst to oil ratio increases the gas oil conversion as well as the coke yield. This is because of the increase in catalyst sites, on which the cracking take place. Although there is an increase in the coke yield, it is not very significant. The increased catalyst to oil ratio also increases the temperature of the riser. But that increase in temperature is moderated by additional cracking, which is due to increased catalyst circulation rate. High C/O ratio favors high gasoline yield.

7. NOMENCLATURE

A_r	Cross sectional area of the riser, m^2
C/O	Cycling catalyst rate/feedstock mass flow rate
CCR	Rate of cycling catalyst kg/sec
$C_{p,c}$	Catalyst heat capacity, kJ/(kg.K)
$C_{p,fl}$	Liquid oil feed heat capacity, kJ/(kg.K)
$C_{p,fv}$	Liquid oil feed heat capacity, kJ/(kg.K)
E	Activation energy, kJ/kmol
F_{rgc}	Regenerated catalyst flow rate, kg/s
F_{sc}	Spent catalyst flow rate, kg/s
F_{tf}	Oil feed flow rate, kg/s
G_F	feed stock mass flow rate kg/s
H	Catalyst hold up, kg
h_c	Specific enthalpy of catalyst, kJ/kg
h_h	Specific enthalpy of hydrocarbon, kJ/kg
ΔH_{evp}	Heat of oil feed evaporation, kJ/kg
H_{lri}	Heat loss from riser, kJ/kg
$k_{i,j}$	Rate constant for the species j involved in the formation of I species, s^{-1}
q_{react}	Heat of reaction per unit volume, kJ/(m^3.s)
R	Gas constant. 8.314 kJ/ (kmol. K)
S	Slip factor, dimensionless
S_v	Space velocity, kg feed/(kg catalyst.s)
T	Temperature, K
t_c	Catalyst residence time, s
t_v	Gas oil space time, s
v_c	Catalyst velocity in bed, m/s
V_R	Volume of riser, m^3
v_v	Gas velocity in bed, m/s
x	dimensionless length of the reactor
y_i	Mass fraction of i^{th} lump in feed stock
z_0	Length of the riser, m

Greek letters

α	Catalyst deactivation constant
ε	Void fraction
Ø	Catalyst activity decay function
θ	Dimensionless time
ρ	Density of gas oil feed kg/m^3
ρ_c	Catalyst density, kg of catalyst /m^3 of bed

Subscripts

c	catalyst
i	hydrocarbons
rgc	Regenerated catalyst
ris	Riser
vap	Vapor

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