The Multi-Objective Optimization of an Actual Hydro Cracking Unit

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In the process of oil refining, hydro cracking is a process through which a heavy hydrocarbon cut is converted into lighter and more valuable products in presence of hydrogen. The current study is concerned with a multi objective optimization of several hydro cracking unit's reactors of the Shazand refinery. In this regard, a tube reactor in a fixed bed has been modeled and the results validated with industrial data collected from the aforementioned refinery. Then the reactor optimized with the aim of increasing production with respect to the least reduction in the catalytic activity and efficiency in terms of hydrogen and fuel gas consumption. The results indicated that, optimization plus changes in operating conditions led to increased or maintained conversions at accepted industrial levels. Furthermore, the procedure to reduce the hydrogen consumption complied with led to an estimated annual reduction of 83,373.84 hNm^3 hydrogen consumptions plus annual saving of about 87,120 Nm^3 in heater's fuel gas consumption. These were economically valuable and in particular, important in terms of environmental issues. Operating parameters varied within ±0.1, ± 0.3, ±0.6, ± 1 and ± 1.2 ºC for the reactor inlet temperature for 5, 10 and 20 % by volume of hydrogen injection into the feed and inlet. Optimal variations ranged for the reactor inlet temperature from - 0.7 to +0.3 °C as well as; for inlet hydrogen injection determined to be + 9 to – 9 % by volume and for the feed inputs were found +4 to 8 % by volume.

1. Introduction

Hydro cracking processes are extremely important for producing valuable products such as naphtha and middle distillates from a wide range of refinery feeds (Bhutani et al., 2006). In more recent years, due to the changing structure of refineries, increased demand for light products such as gasoline as well as; having been faced with new generation of catalysts have all led to rapid development of the hydro cracking processes. In a hydro cracking units high pressure hydrogen is used for producing saturated multi branches hydrocarbons and reducing coke formation on catalyst's surface. In turn, saturated multi branches hydrocarbons increase stability of lighter products like gasoline. Reduction in coke formation on the catalyst surface will enhance catalyst activity and life time (Scherzer and Gruia, 1996). The most important principle in optimizing hydro cracking unit's reactors is to have a valid kinetic model (Bhaskar et al., 2003). To determine the validity of a model, its results may be compared with data from laboratory or industrial scale set ups. In this study a mathematical model results are compared with experimental industrial data from the Shazand refinery then optimized with respect to some objective function. Objective functions might be considered as conversion as well as; hydrogen and fuel gas consumptions. These parameters have been optimized by changing operating conditions such as input temperature, reactor inlet and bed temperatures at certain intervals.

2. Describing hydro cracking unit under consideration

The unit studied utilized hydrogen in vicinity of catalyst under the molecular breakdown process to convert heavy feed intake from vacuum distillation unit into valuable products such as LPG, light naphtha as well as; heavy naphtha, kerosene and gas oil. This unit is composed of two sections including the reactor and product separation. Each reactor consisted of four beds and since reactions were highly exothermic, cooling system of injected hydrogen was used. Feed of this unit was a relatively heavy cut out of the vacuum distillation column's middle cuts. Feed entered the reactor from the upper part and during downward movement the molecular breakdown reactions occurred. General overview of the reactor section of the hydro cracking unit is shown in Figure-1 (Moghadassi et al., 2011).

3. Modeling

3.1 Mathematical modeling of the hydro cracking reactor

Many investigations have been performed on the process kinetics of heavy oil residue from which several models have been developed. Ideally, a kinetic model should consider all reactions due to feed components. In fact, due to complex chemistry of hydrocarbons in the feed and reacting mixture as well as; the large number of components and reactions also the lack of kinetic data; to perform such task would be extremely difficult. On the other hand, main check point parameters refineries are faced with daily are yield and quality, reactor temperature and hydrogen consumption (Rajesh et al. 2001). In this direction, the present study has been performed based upon the hydro cracking knowledge and kinetic model using sensitivity analysis. In other words, using a discrete kinetic model and assuming that the reaction take place in a tubular fixed bed reactor, a mathematical model has been developed and solved utilizing MATLAB 6.2 software. The kinetic model was validated with industrial data available from the abovementioned plant. Thus, concentration and temperature profiles from this model were obtained. Utilizing industrial data of hydro cracking unit, several objective functions such as the conversion as well as; hydrogen and fuel gas consumptions were considered in order to optimize the hydro cracking unit's reactors. To do this the kinetic model with catalyst activity losses from elsewhere (Moghadassi et al., 2010), has been used which is described below.
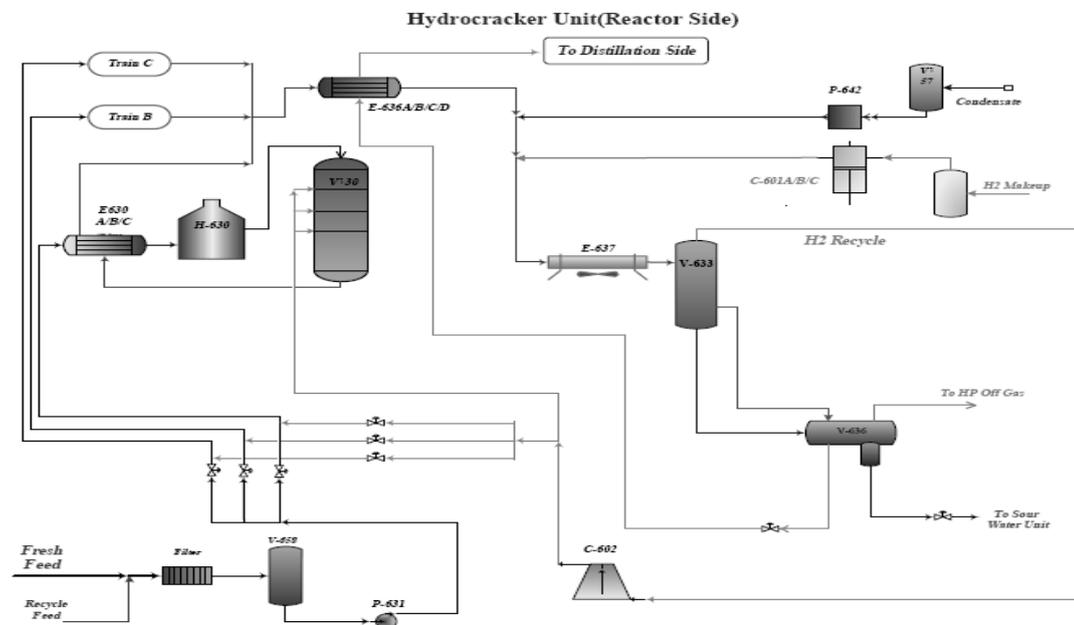

Figure 1: General overview of the reactor section of the hydro cracking unit (Moghadassi et al., 2010)

In hydro cracking process, catalyst activity is defined as the temperature required to obtain a fixed conversion rate under certain specified operating conditions (Boudart and Mariadassou, 1984).

$$\text{activity} = \frac{\text{reaction rate with used catalyst}}{\text{reaction rate with fresh catalyst}} \tag{1}$$

For a simple reaction such as: $A \rightarrow \Pr oducts$; and an nth-order reaction rate then:

$$-r_A = k.C_A^n.a = k_0 e^{-E/RT}.C_A^n.a \tag{2}$$

In order to keep the conversion at the same level, the feed temperature increased when the catalyst activity decreased gradually (Levenspiel, 1972); furthermore:

$$a = e^{\left[-E/R(\frac{1}{T_0}-\frac{1}{T})\right]} \tag{3}$$

Next, to simplify the model, the following assumptions are taken into account.
1. Concentration and temperature are uniform throughout a cross section such that there are no interfaces; hence no such gradients existed in this study
2. The heat capacities of liquid and gas and the heats of reactions were taken to be constant
3. The liquid and vapor phases were at equilibrium and the compositions may be calculated using flash vaporization. Furthermore, the vapor behaved as an ideal gas.
4. Reactor is operating in an adiabatic mode.

Employing the above assumptions, the steady state mass and energy balances with catalyst deactivation function (*a*) might be described as follows:

    i)   Crackable hydrocarbons mass balance:

$$G_t \frac{\partial C_i}{\partial x} = -\rho_i k_i a. C_i \tag{4}$$

    ii)   Hydrogen mass balance:

$$G_t \frac{\partial C_H}{\partial x} = -\alpha \rho_i k_i a C_i \tag{5}$$

    iii)   Heat and energy equation:

$$G_t (c_{p,H} C_H + c_p C_T) \frac{\partial T}{\partial x} = -(\Delta H)\rho_i k_i a. C_i \tag{6}$$

It is also necessary to define the conditions of fluid at the location of quenching:

$$G_{tq} = G_t + G_{gq} + G_{lq} \tag{7}$$

To solve these nonlinear partial differential equations; Runge Kutta method of fourth order was utilized (Nandasana et al., 2003). Therefore, concentrations, temperature and amount profile of consumed hydrogen obtained from solving these equations. Next, utilizing the obtained concentrations in terms of different ratio between them and input concentration, the conversion was determined. It is reminded that; the validation of obtained results done with the data from the Shazand refinery. Ultimately, the optimization of the reactor was performed.

3.2 Modeling results

The results of mathematical modelling of the hydro cracking reactor after validation with industrial data are shown below. A comparison of temperatures predicted by the present model with the data from Shazand refinery is shown in Figure 2. As shown in this figure, the deviation of the model from actual data is less than 5 %, which considering the complexities involved is rather pleasing:
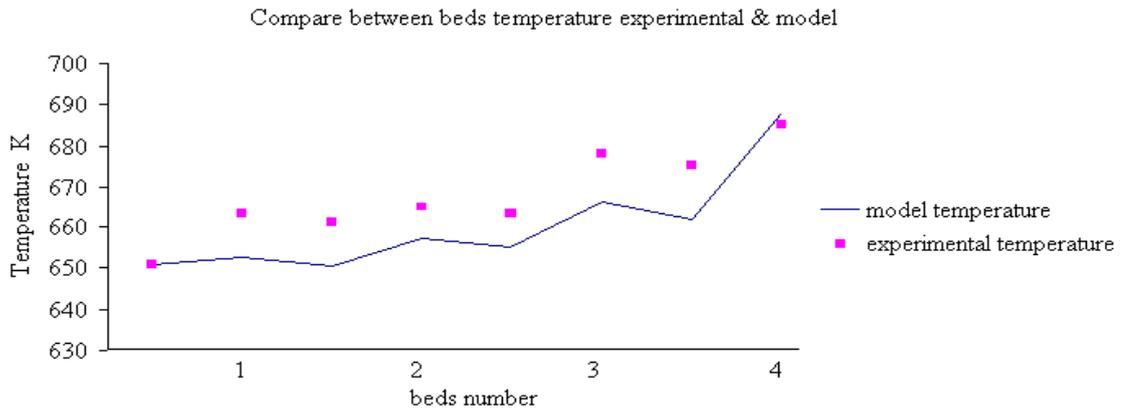

Figure 2: Comparison between the present model and actual Bed temperature

Conversion percent which is representing cracking rate and production; might be one of the most important factors in optimization of this process. Figure 3 showed the predicted conversion by the present model for the reactor of the hydro cracking unit of the Shazand refinery for 3 y. It is noteworthy that, the industrial experimental conversion remained steady at about 97 %.

The deviation of model from the industrial data is less than 5 %. It is reiterated that the conversion deviation was calculated as: $(X_{model} - X_{experimental}) / X_{model}$.
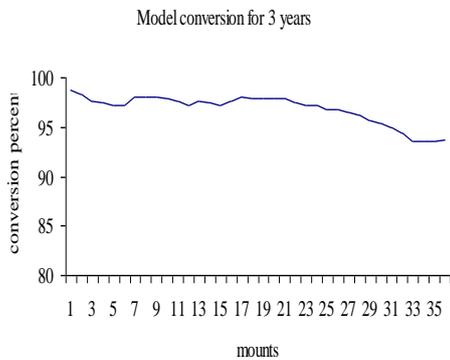

Figure 3: Theoretical amounts of conversion determined from the present model
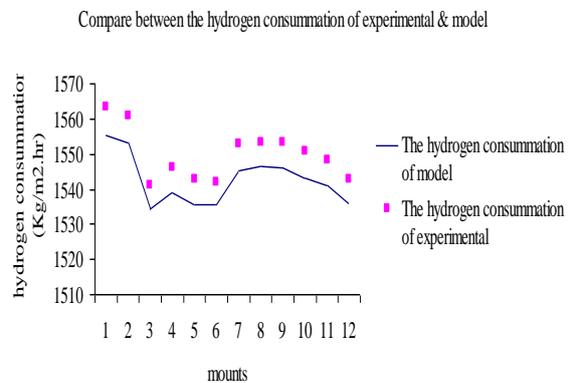

Figure 4: Comparison between rate of hydrogen consumption predicted by the model and its actual value

As may be seen, the deviation of the hydrogen consumption from the actual value was less than 5 % which is an indicative of the relative robustness of the modeling.

4. Optimizing hydro cracking reactor performance

With regards to the information obtained from the sensitivity analysis, a range for hydro cracking reactor optimization might be obtained for three parameters including; the reactor inlet temperature, hydrogen injection into the reactor and reactor feed input. These were done while bearing in mind the conversion, hydrogen injection and reduction of fuel gas consumption were targets of optimizations. Collecting results in the sensitivity analysis section, with respect to aforementioned issues; a pattern for optimizing hydro cracking reactor utilizing above variable parameters was developed in a way to have the most acceptable conversion for an industrial unit. This led to a minimum decrease in the observed catalyst active life. Ultimately, through such optimizations, the most possible economic and environmental savings were achieved. In this study hydrogen consumption was therefore, reduced to about 9.57 kNm^3/h. In other words, annual reduction of about 83,373.84 kNm^3 was made possible. The average conversion in this case was about 97 % which was indeed desirable for an industrial unit. The reason for not exceeding beyond this conversion was the compensation made mostly due the desire of having a minimum loss on catalyst active life.

It is seen through Figure-1 that the reactor feed passed through the heat exchanger and furnace while its temperature raised to 376 $^{\circ}$C before entering the reactor. The heat exchanger inlet temperature is about 152 $^{\circ}$C and its outlet temperature is about 368 $^{\circ}$C while the furnace outlet temperature is about 376 $^{\circ}$C. Heat exchanger inlet temperature was fixed and its outlet temperature was kept variable depending on the requirement of the reactor outlet temperature. If the reactor outlet temperature rose, then the heat exchanger outlet temperature increased and vice a versa. These changes of heat exchanger temperature outlet were calculated rather easily. Calculations showed that for every 0.9 $^{\circ}$C change in the reactor outlet temperature, the heat exchanger outlet temperature changed about 1 $^{\circ}$C. This meant that they were positively correlated.

Next, through changes in the amount of third injecting hydrogen (*i.e.*; to the bottom bed) and using results and considering aforementioned constraints in sensitivity analysis section; an operating algorithm offered to demonstrate that an increase in the reactor outlet temperature of about 0.5 $^{\circ}$C led to the furnace inlet temperature of at most the same amount. This furnace worked with fuel gas to supply the required heat duty. Fuel gas consumption of this furnace was about 180 Nm^3/h indicating that a decrease or increase of 1 $^{\circ}$C would cause a 20 Nm^3/h increase in the fuel gas consumption. Therefore, increasing the reactor outlet temperature by 0.5 $^{\circ}$C led to fuel gas consumption saving of 10 Nm^3/h. In other words, about 8712 kNm^3 annual saving in fuel gas consumption obtained through the scheme developed in this research.Illustrations and tables

5. Conclusions

In this study, an optimization of the reactor of the hydro cracking unit of the Shazand refinery has been performed. This was undertaken baring in mind the necessity of keeping the catalyst durability at high levels as well as; maintaining the steady conversion of the industrial unit. Normally the inlet and also reactor beds temperatures increased in order to compensate conversion reduction. This caused a sharp drop in the catalyst activity hence, regeneration after a while was required. This in turn would be costly since the production process should be halted during catalyst regeneration. Following the resulting patterns in this study, it was concluded that not only the life time of the catalyst enhanced but also the conversion during latter months of the year was higher than its amount at the same time for the normal operation.

Furthermore, through this study it was revealed that, the hydrogen consumption might be reduced by about 83,373.84 kNm^3/y. It is reminded that for producing hydrogen, fuel gas was consumed. Thus, when hydrogen consumption was lowered, the fuel gas consumption decreased as well. This further meant that negative harmful effects on environmental pollutions were downgraded in addition to the economic benefits of such reductions. Ultimately, through changes considered in this research for the amount of third injecting hydrogen (i.e. to the bottom bed) and using results of the sensitivity analysis performed; an operational algorithm offered to decrease annual fuel gas consumption by about 8712kNm^3 which is both economically valuable and environmentally attractive.

Nomenclature

a	activity
C_A	feed concentration in the reactor effluent
C_i	Wight fraction for crack able hydrocarbons
C_{iq}	concentration of crack able hydrocarbons
C_h	Wight fraction for hydrogen
C_{Hq}	concentration of hydrogen
Cp_i	specific heat capacity kJ/kg. K
E	activation energy, kJ/kg
IBP	initial boiling point, ^0C
FBP	final boiling point, ^0C
G_{gq}	gas quenching mixtures
G_{lq}	liquid quenching mixtures
G_T	total mass velocity (liquid & gas)
H	heat of reaction (kJ/kg)
K	overall first-order reaction rate constant for the cracking
R	ideal gas constant
r_A	reaction rate
T	operating reactor temperature, K
T_0	weighted average bed temperature (WABT)
T_q	temperature after the mixing Structure
α	hydrogen consumption coefficient
p	density (kg/m^3)

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