Simulation of naphtha reforming unit using Aspen plus user model

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Abstract
In this study, a semi-regenerative catalyst naphtha reforming process was simulated by linking Aspen plus with reactors modeled in Matlab software. The reason behind the employment of this method is its ability to apply the suitable pressure drop, flow distribution and catalyst characteristic in the naphtha reforming reactor. Because of the deactivation of the catalyst, the effect of time on temperature, furnace heat duty, and mass flow was investigated. The model data was validated with a domestic plant. The deactivation had significant effects on the mass fraction of hydrogen and light end products while the change of other parameters was negligible.

Key words: Simulation, semi-regenerative catalyst naphtha reforming, Aspen plus, use model

Introduction

The production of high octane gasoline in petroleum refineries and petrochemical industries is extensively practiced by catalytic reforming of naphtha. In today's competitive market it is crucial that a catalytic reformer model that can monitor and optimize the performance of the plant for maximum profit would exist. Also, these models could aid with the decision making regarding catalyst process selection.

Naphtha reformers are multibed reactors that operate under moderate pressures (10-40 bar), high temperatures (450-520 °C) and high hydrogen to hydrocarbon molar ratio (5-10) [1]. Bifunctional catalyst like Pt-Re/Al_2O_3 that are used in naphtha reforming have a metal component (Pt-Re) for dehydrogenation of naphthenes to aromatics with high octane number hydrocarbons Eqn ((1) and naphthenes to paraffins Eqn (2) and an acidic component for hydrocracking of paraffins and naphthenes to light ends Eqn ((3(4) [2].

Even with today's technology, it is not practical to identify all the complex hydrocarbon mixtures of naphtha and account for all the reactions they undergo. For this reason, attempts have been made to model naphtha with lumping of the components by carbon number based on similar properties and kinetic behavior. A simple model was developed by smith in which naphtha was lumped to naphthenes, paraffins and aromatic(PNA) [3].

This study aims to develop a method for the investigation of complex processes like naphtha reforming in aspen plus software. This method consists of linking Aspen plus user model block with each bed that was modeled in Matlab software. Because of high the computation time, Smith's reaction network was employed in this study. In this manner, we could investigate the effect of time on different parameters of the plant.

Process description

The schematic diagram for the semi-regenerative catalyst naphtha reforming process is presented in Figure *1*. Stream 1 is mixed with the recycle stream and enters the first furnace were it reaches the desired temperature. Specifications for the inlet stream, catalyst and each bed are gathered from domestic refinery [4]. The tubular reactors operate adiabatically and the chemical reactions take place in the catalytic bed where the naphtha is flowing axially. The furnaces heat the inlet stream of each reactor to the desired temperature. The outlet of the third reactor is fed to the flash separator to adjust H_2 to the hydrocarbon ratio (H_2/HC) for the feed of the first reactor. Stream 5 enters flash block V3 at 30°C and 345 kPa were light hydrocarbons are separated from heavy ones as products.

The method that is used to model the reaction network is presented in equations (1)(4). The kinetic reaction parameters are presented in Bommannan(1989) [2] were the deactivation equation (5) was taken from Khosravanipour(2009) [5].

$$\mathrm{Naphthenes}(C_nH_{2n}) \leftrightarrow \mathrm{Aromatic}(C_nH_{2n-6}) + 3H_2 \quad (1)$$

$$\mathrm{Naphthenes}(C_nH_{2n}) + H_2 \leftrightarrow \mathrm{Paraffins}\ (C_nH_{2n+2}) \quad (2)$$

$$\mathrm{Naphthenes}(C_nH_{2n}) + aH_2 \rightarrow \mathrm{Lighter\ ends}\ (C_1 \sim C_{n-1}) \quad (3)$$

$$\mathrm{Paraffins}(C_nH_{2n+2}) + bH_2 \rightarrow \mathrm{Lighter\ ends}\ (C_1 \sim C_{n-1}) \quad (4)$$

$$\frac{da}{dt} = -K_d \exp\left(\frac{-E_d}{R}\left(\frac{1}{T} - \frac{1}{T_R}\right)\right) a^7 \quad (5)$$

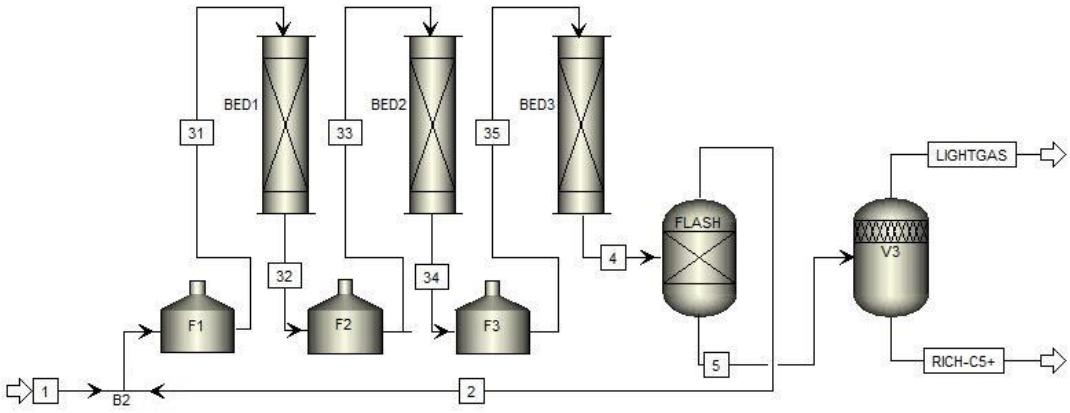

Figure 1. schematic of semi-regenerative naphtha reforming process in aspen plus

These reactors are modeled by the user-model block in Aspen-Plus. Aspen sends the feed data to excel where it is transmitted to Matlab. In this software mass, heat and momentum balance equations were solved with implicit Euler method. Finally, the results were sent to Aspen plus by excel which is shown in Figure *2*.

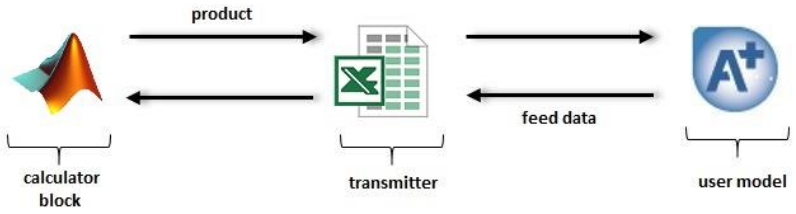

Figure 2. Linking process description

Model validation

The model has been validated with domestic plant data for a steady state conventional tubular reactor. From Table 1 it is evident that there is a great agreement between the data from the plant and model. The temperature for the outlet stream of each reactor has a relative error of less than 1% but the aromatics in the outlet of the third reactor has a relative error of 3.3%.

Table 1. Comparison between plant data and proposed model [4]

stream	plant data		proposed model		
	temperature K	aromatics mole%	pressure kPa	temperature K	aromatics mole%
32	722	-	3566.3	719.89	34.9
34	753	-	3414.5	751.43	47.5
4	770	57.7	3324.9	772.13	55.81

Result and discussion

The effect of time has been investigated for the overall performance of the naphtha reforming process along the length of each reactor bed. The modeling result shows the change of catalyst activity for each bed in its average temperature Figure 3(a). The high temperature effects the average aging time of catalysts, for this reason, the activity of the catalyst in the third reactor has decreased the most relative to other reactors Figure 3(b).

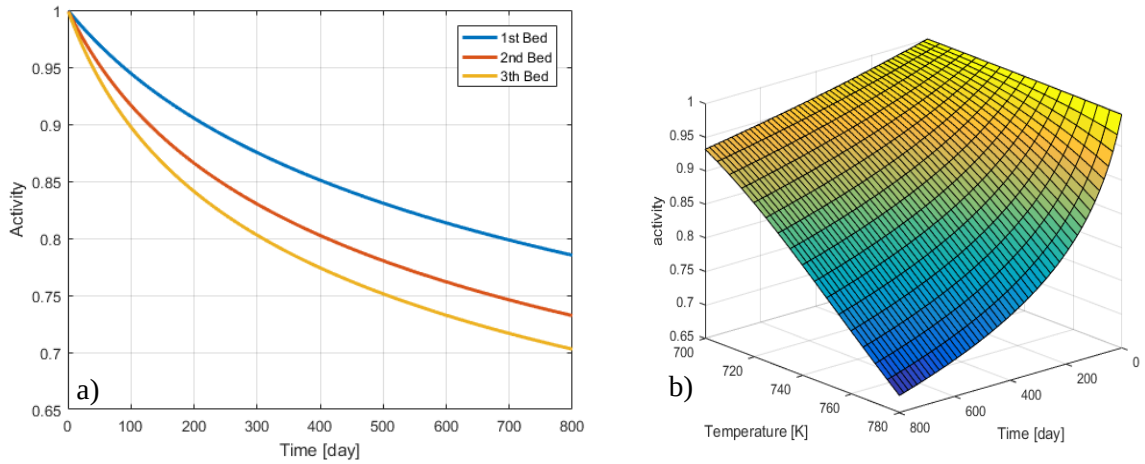

Figure 3. a) The effect of time on average catalyst activity in each bed, b) effect of time and temperature on activity.

The temperature profile along the fixed bed reactor has been illustrated in Figure 4. There is no considerable change in the outlet temperature of three reactors after 800 days.

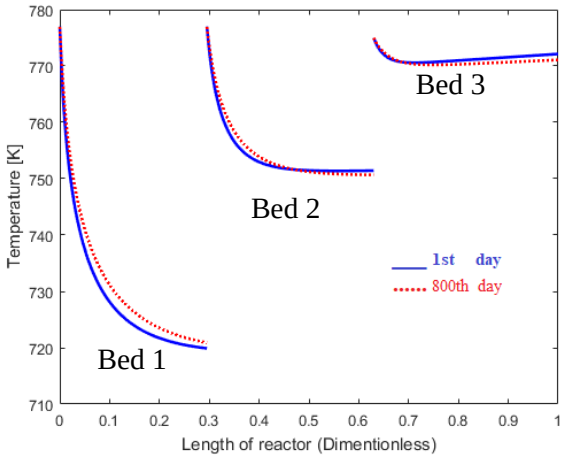

Figure 4. Temperature profile along each bed

The results show there is a slight difference in the heat duty of second and third furnaces. This is shown in Table 2.

Table 2. Effect of time on furnace heat duty

Furnace	F1		F2		F3	
Day	1	800	1	800	1	800
heat duty (MW)	8.0	8.0	3.4	3.3	1.4	1.5

The PNA molar flow versus the dimensionless reactor length is presented in Figure 5(a). As evident from the figure, there is a slight difference between the aromatic production after 800 days which the activity for the third bed is about 0.7. Because the temperature decrease as a result of endothermic reactions the conversion decreases along with the length of the reactors. In the third bed, the consumption of paraffin is higher than the first two reactors. The reason behind this is the decrease of naphthene partial pressure that results in the decrease of paraffin production.

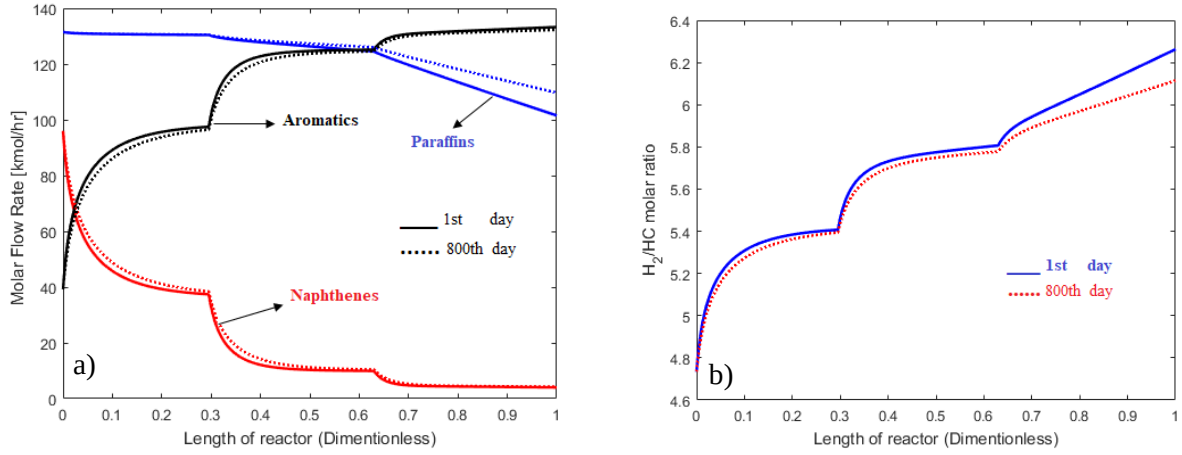

Figure 5. a) Molar flow rate profile along each bed, b) H_2/HC ratio profile along each bed

The ratio of hydrogen to hydrocarbon is an important factor in the deactivation of the catalyst. Figure 5(b) shows the ratio decreases 0.15 after 800 days, although the hydrogen production increases 9.5 kmol/h. so it would be better than the catalyst deactivation equation would encompass this ratio is well.
The results for light gas and rich C_5^+ from the flash block in Aspen plus are presented in Table 3. The main difference after 800 days is the mass fraction of hydrogen and light ends components in the light gas stream. Also, its total mass flow has decreased by 704 kg/hr after 800 days. Consequently, the mass flow has increased in the rich C_5^+ reformate stream by 690 kg/hr which major part of this is attributed to unreacted paraffins after 800 days.

Table 3. Stream results

parameter	stream 5		stream light gas		stream C5+ reformate	
day	1	800	1	800	1	800
Ftotal (kg/hr)	30214.3	30199.8	3425.98	2721.32	26788.3	27478.5
weight fraction						
w_PC5+	0.385155	0.416672	0.028454	0.037776	0.42909	0.452951
w_NC5+	0.015006	0.016002	0.000454	0.000594	0.016819	0.0174768
w_AC6+	0.470135	0.467173	0.023912	0.029142	0.525745	0.509112
w_H2	0.015455	0.016178	0.139436	0.185106	3.50E-06	3.79E-06
w_LE	0.114249	0.083946	0.807744	0.747402	0.027824	0.020457

Conclusion

In this study, Aspen plus user model was employed with Matlab and Excel to investigate the effect of time on temperature, pressure, activity and mass flow profile in the length of each bed. It was observed that the deactivation of catalysts did not significantly affect the temperature drop and a result the heat duty of the second and third furnaces. Also, the pressure drop did not significantly change after 800 days. But the main difference is the production of light gas and rich C_5^+ streams in the V3 flash block outlet. In the light gas stream, there was 704 kg/hr increase in mass flow and the mass fraction of hydrogen had increased from 0.139 to 0.185. The light end mass fraction in the same stream has decreased from 0.808 to 0.747. The reason behind the increase of paraffin mass fraction in rich C_5^+ stream is a result of unreacted paraffin accumulating the plant after 800 days.

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