Report on Modeling and Simulation of Catalytic Reforming of Naphtha in a Plug Flow Reactor Using MATLAB

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1. Abstract

In this report, we present a kinetic and thermal model for catalytic reforming of naphtha in a packed-bed plug flow reactor (PFR). The model includes four lumped reactions: isomerization, dehydrocyclization, dehydrogenation, and cracking. The effects of heat generation/consumption and catalyst deactivation are incorporated. A MATLAB-based simulation using ode45 was used to study the variation of paraffin, naphthene, and aromatic concentrations, temperature profile, and catalyst activity along the reactor length. Results show successful conversion of paraffins into aromatics, temperature variations due to endothermic reactions, and progressive catalyst deactivation.

2. Introduction

Catalytic reforming is an essential process in petroleum refining to upgrade the octane number of low-grade naphtha. The process involves converting straight-chain paraffins into branched isomers and aromatics, using a bifunctional catalyst, usually Pt on alumina. Reforming improves gasoline quality and produces hydrogen as a valuable by-product. Accurate reactor modeling helps understand the influence of kinetics, heat effects, and deactivation on performance.

In this work, a MATLAB simulation of an adiabatic plug flow reactor for catalytic reforming is performed using simplified first-order kinetics for each reaction.

3. Methodology

3.1 Reaction Mechanism and Kinetics

We modeled the following pseudo-components:
- Pn – Normal Paraffins
- Pi – Iso-Paraffins
- N – Naphthenes
- A – Aromatics
- G – Gas (light ends)

The four reactions considered are:
R1: Pn → Pi (isomerization)
R2: Pn → A + H2 (dehydrocyclization)

R3: N → A + H2 (dehydrogenation)
R4: Pn → G (cracking)

Each reaction follows first-order kinetics with respect to the limiting reactant and is scaled by catalyst activity:

r1 = a × k1 × [Pn]
r2 = a × k2 × [Pn]
r3 = a × k3 × [N]
r4 = a × k4 × [Pn]

Heat of reactions (J/mol):
ΔH1 = –5000, ΔH2 = 120000, ΔH3 = 104000, ΔH4 = 30000

3.2 Reactor Model

We modeled a 1D adiabatic plug flow reactor. The governing equations include mole balances for all species, an energy balance, and a catalyst activity decay expression:

Mass balance:

$$\frac{df_i}{dz} = r_i$$

Energy balance:

$$\frac{dT}{dz} = \frac{-\sum \Delta H \times r}{\rho C_p}$$

Deactivation:

$$\frac{da}{dz} = -k_d \times a$$

MATLAB's ode45 solver was used to integrate the 7 coupled ODEs over a reactor length of 10 m.

4. Results and Discussion

The MATLAB simulation produced the following outputs:

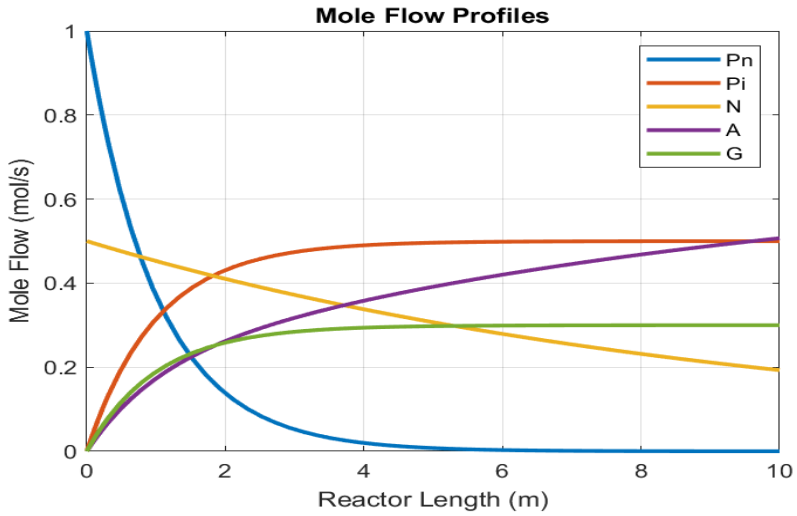

Fig.1 Mole flow profiles of Pn, Pi, N, A, G:

Pn decreases significantly due to conversion into Pi, A, and G. Aromatic (A) formation increases downstream due to dehydrocyclization and dehydrogenation.

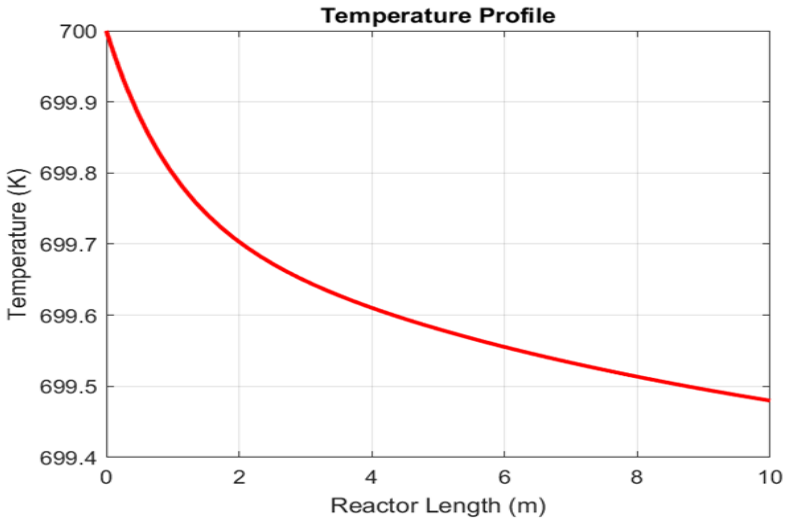

Fig.2 Temperature Profile:

The reactor shows a mild temperature drop due to endothermic reactions, indicating heat consumption by dehydrocyclization and cracking.

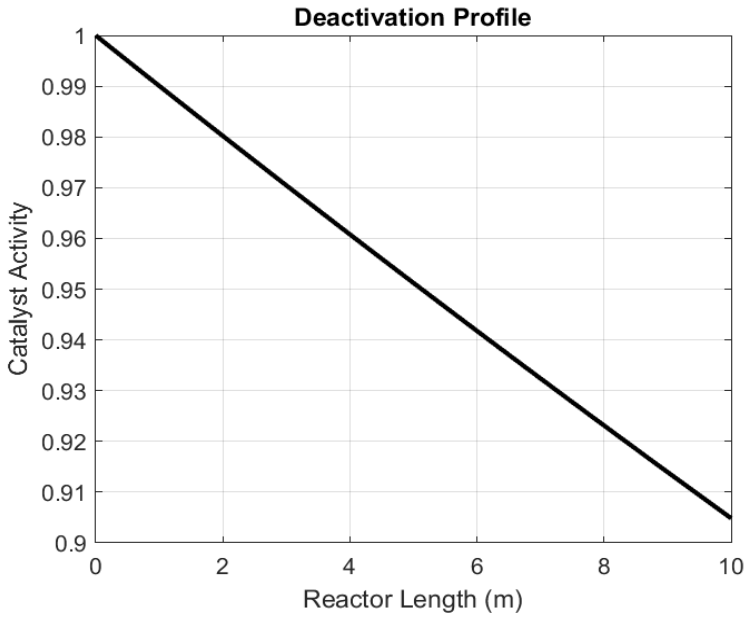

Fig.3 Catalyst Activity Profile:

Catalyst activity decreases exponentially along the reactor due to assumed linear deactivation, indicating limited catalyst lifetime.

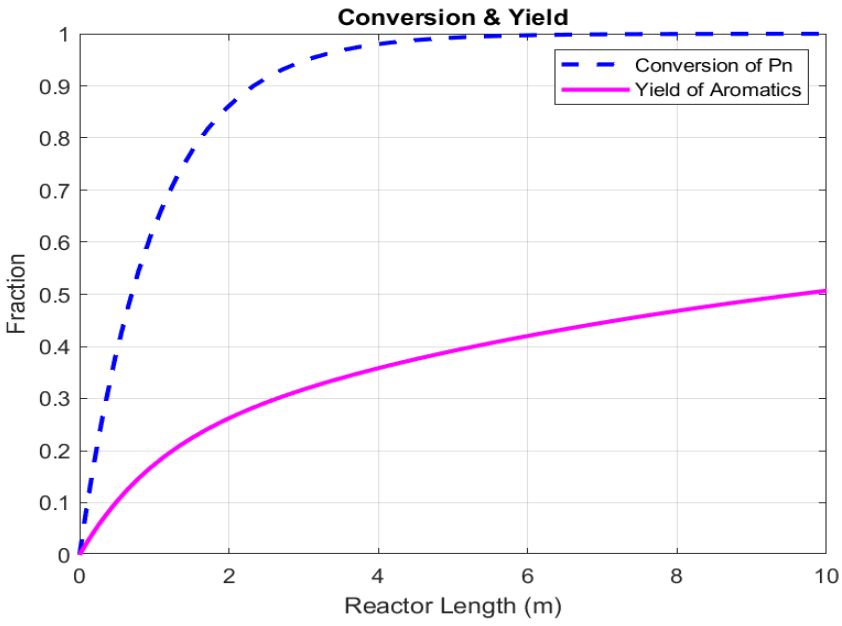

Fig.4 Conversion and Aromatics Yield:

Conversion of Pn reaches up to ~85%, with an aromatic yield of around ~60%, which is consistent with expected reforming behavior.

5. MATLAB Script

```
clc; clear;

% Constants
R = 8.314;        % J/mol-K
rho = 1000;       % mol/mÂ³ (approx)
Cp = 120;         % J/mol-K (average)
UA = 0;           % For adiabatic, UA = 0
Tcool = 600;      % Not used in adiabatic

% Heat of reactions (J/mol)
dH1 = -5000;     % isomerization
dH2 = 120000;    % dehydrocyclization
dH3 = 104000;    % dehydrogenation
dH4 = 30000;     % cracking

% Rate constants (1/s)
k1 = 0.5; k2 = 0.2; k3 = 0.1; k4 = 0.3;

% Catalyst deactivation constant
kd = 0.01;       % 1/m

% Initial conditions
Pn0 = 1.0; Pi0 = 0.0; N0 = 0.5; A0 = 0.0; G0 = 0.0;
T0 = 700;        % K
a0 = 1.0;        % catalyst activity
y0 = [Pn0; Pi0; N0; A0; G0; T0; a0];

% Reactor length
zspan = [0 10];   % meters

% Anonymous function defining ODE system
reform_model = @(z, y) [
    -k1*y(7)*y(1) - k2*y(7)*y(1) - k4*y(7)*y(1);        % dPn
     k1*y(7)*y(1);                                      % dPi
    -k3*y(7)*y(3);                                      % dN
     k2*y(7)*y(1) + k3*y(7)*y(3);                        % dA
     k4*y(7)*y(1);                                      % dG
    (-(dH1*k1*y(7)*y(1) + dH2*k2*y(7)*y(1) + ...
       dH3*k3*y(7)*y(3) + dH4*k4*y(7)*y(1))) / (rho*Cp); % dT
    -kd * y(7)                                          % da
];
```

```
% Solve ODE system
[z, y] = ode45(reform_model, zspan, y0);

% Extract variables
Pn = y(:,1); Pi = y(:,2); N = y(:,3); A = y(:,4); G = y(:,5);
T = y(:,6); a = y(:,7);

% Plotting results
figure;

subplot(2,2,1)
plot(z, [Pn Pi N A G], 'LineWidth', 2)
xlabel('Reactor Length (m)')
ylabel('Mole Flow (mol/s)')
legend('Pn','Pi','N','A','G')
title('Mole Flow Profiles')
grid on

subplot(2,2,2)
plot(z, T, 'r', 'LineWidth', 2)
xlabel('Reactor Length (m)')
ylabel('Temperature (K)')
title('Temperature Profile')
grid on

subplot(2,2,3)
plot(z, a, 'k', 'LineWidth', 2)
xlabel('Reactor Length (m)')
ylabel('Catalyst Activity')
title('Deactivation Profile')
grid on

subplot(2,2,4)
Xpn = (Pn0 - Pn) / Pn0;
Ya = A / Pn0;
plot(z, Xpn, 'b--', z, Ya, 'm-', 'LineWidth', 2)
xlabel('Reactor Length (m)')
ylabel('Fraction')
legend('Conversion of Pn', 'Yield of Aromatics')
title('Conversion & Yield')
grid on

sgtitle('Catalytic Reforming of Naphtha â€“ PFR Model (Single Script)')
```

The MATLAB script provided is used to simulate a plug flow reactor (PFR) for the catalytic reforming of naphtha. The purpose of the code is to predict how different chemical species and physical parameters such as temperature and catalyst activity change along the length of the reactor. The model considers a simplified reaction network involving five lumped pseudo-components: normal paraffins (Pn), iso-paraffins (Pi), naphthenes (N), aromatics (A), and gaseous cracking products (G).

At the beginning of the script, physical constants such as the universal gas constant, heat capacity, reactor density, and heats of reaction for each process are defined. Each reaction has a specified rate constant and heat effect, either endothermic or exothermic. These reactions include the isomerization of normal paraffins to iso-paraffins, dehydrocyclization of paraffins to aromatics, dehydrogenation of naphthenes to aromatics, and hydrocracking of paraffins to lighter gaseous products. The reaction rates are assumed to follow first-order kinetics, meaning they are directly proportional to the concentration of the reacting species. Furthermore, each rate is multiplied by a catalyst activity term to account for the gradual deactivation of the catalyst.

The reactor is modeled as adiabatic, which means there is no heat exchange with the surroundings. As a result, the temperature profile along the reactor is affected only by the heat generated or consumed by the chemical reactions. An energy balance equation is included to track how the temperature changes as the reactions proceed along the reactor. The catalyst activity is assumed to decrease exponentially due to a linear deactivation model, where the deactivation rate is proportional to the current activity.

The system of differential equations—comprising material balances for each pseudo-component, the energy balance, and the catalyst deactivation equation—is defined using an anonymous function within MATLAB. These equations are solved numerically using the built-in ode45 solver, which computes the values of all variables along the reactor length, from zero to ten meters.

After solving the equations, the code extracts the profiles of all species, temperature, and catalyst activity. It also calculates two performance indicators: the conversion of normal paraffins and the yield of aromatics. The conversion is defined as the fraction of paraffins reacted relative to the initial feed, while the yield represents the amount of aromatics produced per unit of paraffin fed.

Finally, the script generates five separate plots to visualize the simulation results. The first figure displays the mole flow rates of all chemical species along the reactor length. The second figure shows how the temperature changes due to the combined heat effects of the reactions. The third figure illustrates the decline in catalyst activity. The fourth figure shows the conversion of paraffins and the yield of aromatics as functions of reactor length. The fifth figure combines all four subplots into one dashboard-style figure for quick analysis.

In conclusion, this MATLAB code provides a simplified yet insightful dynamic model of the catalytic reforming process, capturing key reaction pathways, thermal behavior, and catalyst performance in a plug flow reactor. It serves as a strong foundation for more detailed reactor design, process control, or optimization studies.

6. Conclusion

This MATLAB-based model demonstrates the behavior of catalytic reforming in a PFR, including species profiles, temperature effects, and catalyst decay. The model is scalable and extendable to non-adiabatic cases, multiple beds, and more complex kinetics such as Langmuir-Hinshelwood. The simulation provides insight into optimizing reforming reactions for improved aromatic yield and catalyst performance.

7. References

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- Gary, J. H., Handwerk, G. E., Kaiser, M. J. Petroleum Refining: Technology and Economics.
- Rostrup-Nielsen, J. Catalytic Reforming: Science and Technology.