

# The Real-Time Dynamic Modeling and Simulation of Reforming Moving-Bed Reactor

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**Abstract:** This paper proposes a modeling approach to the continuous reforming reactor of broad components, with the consideration of both accuracy and validity it can be used for the dynamic simulation and on-line optimal control. The simulation results of the reforming reactor model are also given.

**Key words:** continuous reforming; dynamic simulation

## 重整移动床反应器实时动态建模与仿真

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**摘要:** 本文根据实时仿真和在线优化控制的需要, 针对宽馏份连续重整反应器, 提出了兼顾“模型的精确性”与“方法的有效性”的一种复杂过程对象数学模型的建立方法, 并给出了模型运行的结果。

**关键词:** 连续重整; 动态仿真

## 1 Introduction

Along with the development of industrial process automation and the enhancement of its complexity, the system analysis and synthesis, which is based on the traditional mathematical model, is getting increasingly difficult. It is always a crucial issue for the research on control theory in pursuing new methods for system modeling<sup>[1]</sup>. The process system is complicated and uncertain, and its modeling is an important problem in the way of process design, optimal control, programming and management, and simulation training.

Continuous reforming process is one of the main devices for petroleum refinement. In this field there are now a lot of reaction dynamic models based on lumping theory, such as Smith's model, Wolff's model, Kmak's model and thirteen lumping model of Mobil Company<sup>[2]</sup>. However, before their structure and dynamic parameters are determined, the experimental tests of complicated reaction dynamics must be done for the models. It costs a great deal to meet the need of the real-time simulation and the on-line optimal control. Therefore, based on the mechanism of reforming reaction, this paper suggests an engineering method of using identification

theory in the description of process system dynamic behavior. This method, combining the chemical mechanism with the identification theory, not only compensates for the disadvantage of the chemical mechanism in the engineering application, but also provides a new idea to complete the description of chemistry reaction behavior for unclearly known mechanism.

## 2 Modeling process

The basic idea of real-time dynamic modeling and simulation of complicated process system is: Basing ourselves on the mechanism of the complicated process, we design a basic framework of mathematical model with the methods of lumping theory and model reduction. Then, by means of heuristic system identification we make use of the process designing data and the experimental data to obtain model parameters and to build practical real-time simulation model. When this method is used in an on-line optimal control, an on-line identification is needed to constantly improve the model accuracy. The idea is expressed in detail as follows. At first, a mechanism analysis of the chemical process is done and, based on the mechanism analysis, a basic framework of mathematical model is designed. Secondly we obtain

model parameters by system identification. Thirdly real-time simulation program is built and model debugging is done. Simulation results are compared with technological data to correct the key parameters. Finally the mathematical model is dynamically debugged and compared with the field data. If model accuracy requirement is not satisfied (dynamic error < 5%, steady state error < 3%), then we will correct the key parameters and do another debugging until the accuracy requirement is met.

Taking into consideration the research results of the real-time dynamic simulation system of continuous reforming technology of broad components, the paper deals with, in detail, the dynamic modeling and simulation of the continuous reforming reactor of broad components.

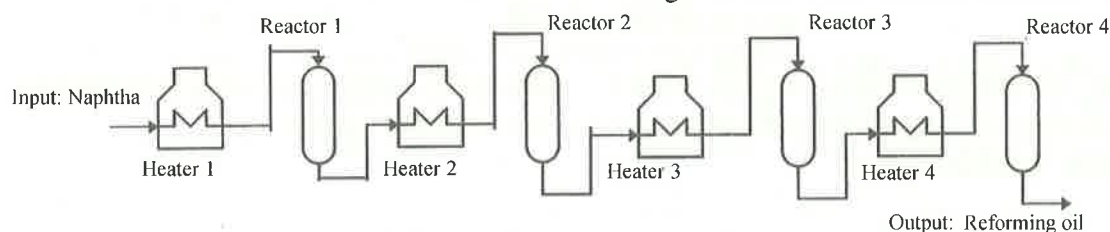


Fig. 1 Diagram of technological process of the continuous reforming reactor of broad components

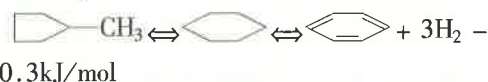
octane petrol and aromatic hydrocarbon. Fig. 1 is the flow sketch chart.

### 3.2 Reacting principle

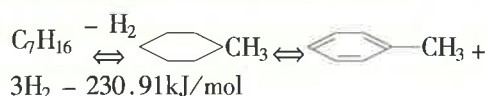
1) Dehydrogenation of cycloparaffin hydrocarbon:



2) Isomeric dehydrogenation of cycloparaffin hydrocarbon:



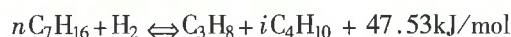
3) Dehydrogenation cyclization of alkane:



4) Isomerization:



5) Cracking hydrogenation:



### 3.3 Model structure of the continuous reforming reactor

In order for the mathematical model describing the continuous reforming reaction process to compromise its accuracy and validity, at first we obtain the basic structure framework of the model based on the reacting principle. We make some reasonable hypotheses to solve the

## 3 Modeling of the continuous reforming reactor of broad components

### 3.1 Technological background

The purpose of the continuous reforming of naphtha is to produce high-octane reforming oil (gasoline), aromatic hydrocarbon and byproducts of gas with abundant hydrogen.

After the pretreated refined naphtha is heated up to become oil steam beforehand in the heater which is connected with all the reactors, the oil steam passes through the reactor containing catalysts with a certain rate. Under the catalysis hydrocarbon molecules of naphtha are rearranged to form a new molecule structure, that is, high-

problem without damaging the accuracy of its external properties.

1) The reactions are unilateral, that is, there is no reverse reaction, and the chemical reaction process takes place in the state of gas only.

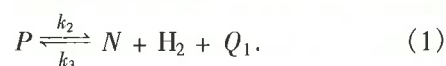
2) The substance flows are all advection.

3) The reacting substance in a sampling period can reach reacting balance in the next sampling period.

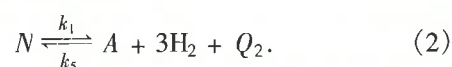
4) System properties approximately obey the one-level reaction system of single molecule.

Based on the hypotheses above, and according to the lumping theory, the reforming substance is divided into four lumpings: aromatic hydrocarbon  $A$ , cycloparaffin hydrocarbon  $N$ , alkane  $P$  and gaseous hydrocarbon  $G$ . The following reactions take place among the lumpings ( $Q_i$  is a reaction heat with sign):

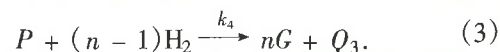
Dehydrogenating cyclization:



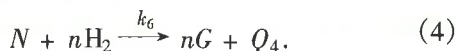
Cyclization reaction:



Cracking hydrogenation:



Cracking hydrogenation:



• Substance continuity equation of each component;

Description in the form of matrix:

$$\frac{d\alpha}{dV} = \Phi K \alpha. \quad (5)$$

In the equation above,

$\Phi$ : activity function of catalyst combined with absorption balance;

$K$ : velocity constant matrix, it is a  $4 \times 4$  matrix;

$\alpha$ : The composed vector of lumping's components denoted are by weight fraction, that is,  $\alpha = [N \ P \ A \ G]^T$ . According to the reaction Equations (1) ~ (4), the form of velocity constant matrix is:

$$K = \begin{bmatrix} -\sum_{j=2}^4 K_{j1} & K_{12} & K_{13} & K_{14} \\ K_{21} & -\sum_{\substack{j=1 \\ j \neq 2}}^4 K_{j2} & K_{23} & K_{24} \\ K_{31} & K_{32} & -\sum_{\substack{j=1 \\ j \neq 3}}^4 K_{j3} & K_{34} \\ K_{41} & K_{42} & K_{43} & -\sum_{j=1}^3 K_{j4} \end{bmatrix} = \begin{bmatrix} -(k_1 + k_2 + k_3) & k_2 & k_5 & 0 \\ k_3 & -(k_2 + k_4) & 0 & 0 \\ k_1 & 0 & -k_5 & 0 \\ k_6 & k_4 & 0 & 0 \end{bmatrix}, \quad (6)$$

where velocity constant  $k_i$  has the form of Arrhenius Equation<sup>[3]</sup>:

$$k_i = k_{0i} e^{-E_i/RT}. \quad (7)$$

The frequency factor  $k_{0i}$  and the activity energy  $E_i$  are identified or simulated according to the experience value and the data of substance balance. In the equation above;  $T$  is the temperature in the reaction.

According to hypothesis (4), the change rate of gasoline is defined by the following equation:

$$r = \frac{\Delta n_p + \Delta n_N}{n_{p0} + n_{N0}}, \quad (8)$$

where  $\Delta n_p$  is the mola number of changed alkane  $P$  in the reaction;  $\Delta n_N$  is the mola number of changed cy-

cloparaffin hydrocarbon  $N$  in the reaction;  $n_{p0}$  is the mola number of alkane in the input substance;  $n_{N0}$  is the mola number of cycloparaffin hydrocarbon in the input substance.

The production rate of gasoline is defined by the following equation:

$$x = \frac{\Delta n_A}{\Delta n_p + \Delta n_N}. \quad (9)$$

In the equation above;  $\Delta n_A$  is the mola number of alkane  $P$  and cycloparaffin hydrocarbon  $N$  that have been changed into aromatic hydrocarbon  $A$  when the reactions achieve balance.

• Heat balance equation:

$$-\frac{dT}{dV} = [-(k_1 - k_5)Q_2 - (k_2 - k_3)Q_1 - k_4Q_3 - k_6Q_4]/C_p. \quad (10)$$

In the equation above:  $Q_1, Q_2, Q_3, Q_4$  are reacting heats of reaction (1) ~ (4) respectively;  $C_p$  is the specific heat;  $V$  is the weight load of catalyst.

• Activity function of catalyst  $\Phi$ :

According to the Langmuir-Hinshelwood formula, we obtain the equation of activity function  $\Phi$  of catalyst as follows:

$$\Phi = \frac{\left(\frac{P_T V_C}{FRT}\right) K_\Phi}{[1 + K_{H_2} \cdot P_{H_2} + \frac{P_T \cdot F_C}{F} \cdot K_\alpha]}. \quad (11)$$

In the equation above;  $P_T, P_H$  are the total pressure and the partial pressure of hydrogen respectively;  $V_C$  is the volume of total catalyst;  $F$  is the total molar flow rate;  $F_C$  is the weight flow rate of input hydrocarbon;  $K_{H_2}$  is the absorption balance constant;  $K_\Phi$  is the real-time velocity constant;  $\alpha$  is the composite vector of lumping components;  $K$  is the absorption balance constant of lumping components.

• The reduced pressure between bed layers of the reactor. The reduced pressure of reactor is also an important variable reflecting the velocity of reaction. We compute the reduced pressure according to Ergun Equation<sup>[3]</sup>:

$$\left(\frac{\Delta P}{\rho \mu_m^2}\right) \left(\frac{d_s}{L}\right) \left(\frac{\epsilon_B^2}{1 - \epsilon_B}\right) = \frac{150}{R_{em}} + 1.75. \quad (12)$$

In the equation above:  $R_{em} = d_s \rho \mu_m / \mu (1 - \epsilon_B)$ ;  $d_s$  is the relative diameter of the surface;  $L$  is the height of reactor;  $\mu_m$  is the average flow rate;  $\rho$  is the density of

liquid;  $\Delta P$  is the reduced pressure between the bed layers. The pressure at reactor exit  $P_2 = P_1 - \Delta P$ ; In the equation,  $P_1$  is the pressure at the top of reactor, and  $P_2$  is the pressure at the bottom of the reactor.

### 3.4 Acquire model parameters and on-line correct models

Based on the mechanism models above, we compute most of the model parameters according to the data of process design and the principle of chemical engineering. As for the part of model parameters that can not be figured out only according to the design data, we obtain them by identifying running data. In order to make a further improvement for the model accuracy to meet the need of application, on-line correction of the model must be done for some times. The steps and methods for the correction are:

#### 1) Disposal of process information.

Making use of the error  $e(t)$  and the change rate of error  $\dot{e}(t)$  between the model output and the plant output, we use the integral rule to reflect the degree of model accuracy. According to the process characteristic and the experience of experts on process, we divide the running load of process into some sections. We can establish present running section of process according to the input of the plant.

#### 2) Correction decision.

The mathematical model above is a non-linear model partly derived from the mechanism and partly from the experience. It gets to a certain accuracy and can meet the real-time need<sup>[4]</sup>. Because the model is described in obvious equations of distributed parameters, the compensations include dynamic compensation and static compensation and the elementary functions of independent variables are used as compensative terms.

At first we define the dynamic attribute of the  $i$ -th model output below:

$$R_{Di} = 100 \cdot \frac{\int_0^T \dot{e}_i^2(t) dt}{\int_0^T y_i^2(t) dt}, \quad i = 1, 2, \dots, m, \quad (13)$$

where  $y_i(t)$  is the measuring value of the  $i$ -th process variable;  $\dot{e}_i(t)$  is the derivative of  $\tilde{y}_i(t) - y_i(t)$ ;  $\tilde{y}_i(t)$  is the corresponding value of model variable;  $T$  is

the time in which the dynamic process stays in the load section.

We define the static attribute of the  $i$ -th model output below:

$$R_{Si} = 100 \cdot \frac{\int_0^{T_s} e_i^2(t) dt}{\int_0^{T_s} y_i^2(t) dt}, \quad i = 1, 2, \dots, m, \quad (14)$$

where  $e_i(t) = \tilde{y}_i(t) - y_i(t)$ ;  $T_s$  is the time in which the process is regulated from the lower limit to the present balance state.

The correction decision is thus given as follows:

When  $R_{Di} < 1$  and  $R_{Si} < 0.5$ , project a) is selected; When  $1 \leq R_{Di} < 10$ , project b) is selected; When  $R_{Di} \geq 10$  or  $R_{Si} \geq 5$ , project c) is selected; When  $0.5 \leq R_{Si} < 5$ , project d) is selected. The project a), b), c) and d) are respectively described below.

a) The requirement of the model accuracy is satisfied, so there is no need to alter the coefficients of the compensative function.

b) The dynamic accuracy of the model is not satisfied, so it is necessary to correct the coefficients of dynamic compensative function.

The form of dynamic compensative function is  $g(\Delta x)$  or  $e^{g(\Delta x)}$ , and  $g(\Delta x)$  is a uniform function of  $\Delta x$ , that is, when  $\Delta x = 0$ ,  $g(\Delta x) = 0$ . Where  $\Delta x = [\Delta x_1, \Delta x_2, \dots, \Delta x_n]^T$ ,  $\Delta x_i$  is the increment of  $x_i$  between two adjacent sampling points.

c) The process is in the state of malfunction or the model cannot meet the needs. It is necessary to dispose the practical process operation or to remodel the process.

d) The static accuracy of the model is not satisfied, then it is needed to correct the gain or the coefficients of the static compensative function. We use  $f(x)$  or  $e^{f(x)}$  as the form of the compensative function in the steady state. Where  $x = [x_1, x_2, \dots, x_n]^T$ , and the detailed form of the function is determined according to the knowledge of the experts on process control.

### 3.5 Model simulation results

We associated the corrected mathematical model above with the real dynamic simulation system to do a simulation experiment according to the operational steps of the practical equipment. The results of the main pa-



rameters are printed as Fig.2(a) ~ Fig.2 (g) below.

After tesing the simulation results above with the

running results of the practical equipment, the testing group of the appraisalment conference believes that the

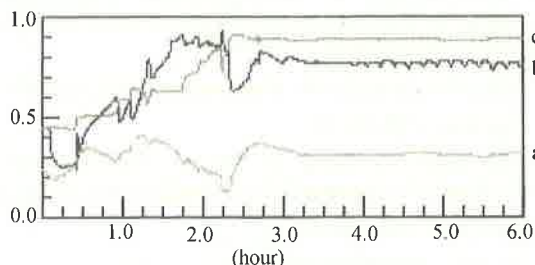


Fig. 2 (a) Naphtha input parameter  
a: Pressure (KCG) (4,5,6);  
b: Temperature ( $^{\circ}$ C) (300,500);  
c: Flow (KG/h) (0,100000).

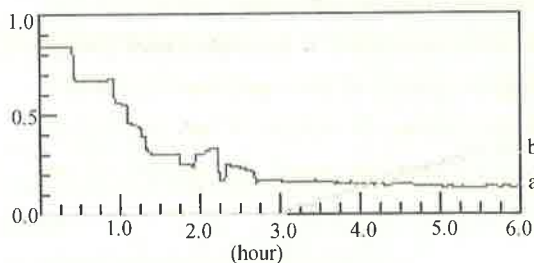


Fig. 2 (b) Naphtha input parameter  
a: Percentage of  $H_2$  (%) (0.25);  
b: Percentage of gasoline (%) (0,10).

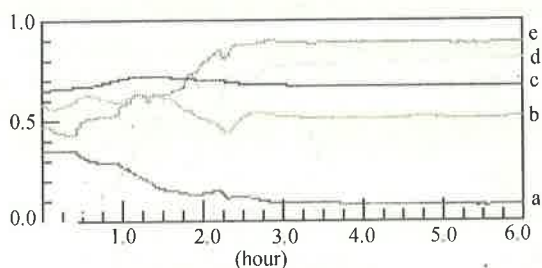


Fig. 2 (c) R201 output parameter  
a: Percentage of  $H_2$  (%) (0.60);  
b: Pressure (KCG) (3,6);  
c: Temperature ( $^{\circ}$ C) (0.600);  
d: Percentage of gasoline (%) (0,100);  
e: Flow (KG/h) (0,100000).

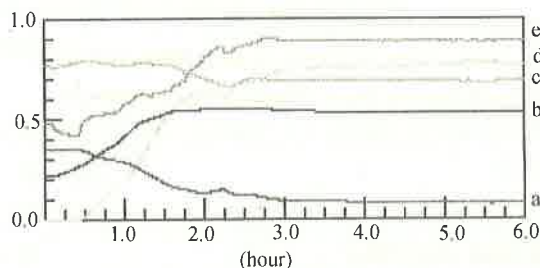


Fig. 2 (d) R201 output parameter  
a: Percentage of  $H_2$  (%) (0.60);  
b: Temperature ( $^{\circ}$ C) (300,600);  
c: Pressure (KCG) (0,6);  
d: Percentage of gasoline (%) (0,100);  
e: Flow (KG/h) (0,100000).

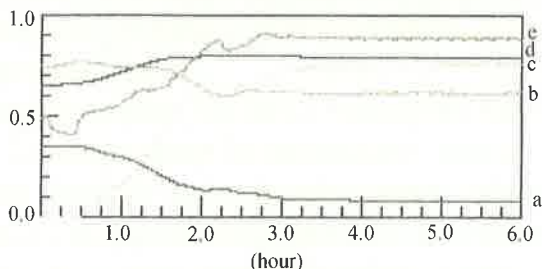


Fig. 2 (e) R203 output parameter  
a: Percentage of  $H_2$  (%) (0,60);  
b: Pressure (KCG) (0,6)  
c: Percentage of gasoling (%) (0,100);  
d: Temperature ( $^{\circ}$ C) (0,600)  
e: Flow (KG/h) (0,100000)

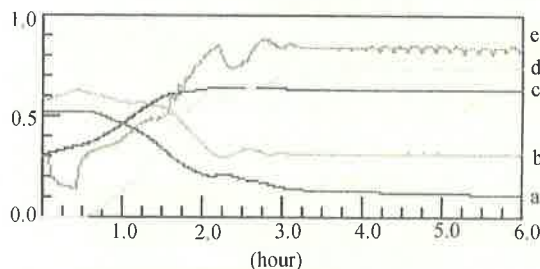


Fig. 2 (f) R203 output parameter  
a: Percentage of  $H_2$  (%) (0,40);  
b: Pressure (KCG) (2,6)  
c: Temperature ( $^{\circ}$ C) (300,600);  
d: Percentage of gasoline (%) (0,100)  
e: Flow (KG/h) (30000,100000)

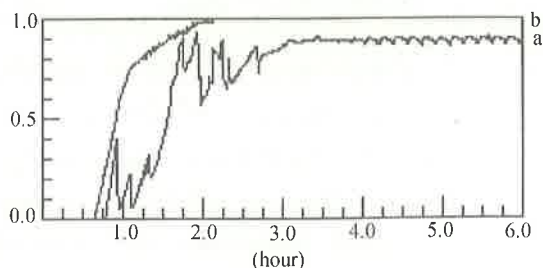


Fig. 2 (g) Change rate and produce rate  
a: Produce rate of gasoline (%) (30,100);  
b: Change rate of naphtha (%) (50,100)

maximum model dynamic error is less than 5% ,and the

error is less than 2% when the process is running in the steady state. The running period of the model is about 10ms ( the type of the computer is 586/166 ), and this index completely satisfies the requirement of the real-time simulation and on-line optimal control.

## 4 Conclusion

In this paper we have introduced a building process of the mathematical model aiming at the real-time simulation and the on-line optimal control of the process system. The continuous reforming technological mathemati-

cal model which is built according to this method has successfully applied in the broad components continuous reforming real-time dynamic simulation system of a certain petrochemical corporation. It has contributed greatly to the simulative running of the equipment's practical running and the training of workers. It has received its user's high praise and had passed the appraisal of the ministry level.

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