

Building a Kinetic Model for Steam Cracking by the Method of Structure-Oriented Lumping

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A kinetic model for steam cracking has been developed by representing feedstock molecules and constructing reaction networks with the structure-oriented lumping method, calculating the reaction rate constant with Materials Studio software, and solving kinetic differential equations with a fourth–fifth-order Runge–Kutta algorithm. A total of 7 structure vectors and 74 reaction rules have been designed to describe molecular composition and their reactions. The model can predict product distribution of different light-oil steam-cracking processes at various operating conditions. Simulation results indicated that predicted data agreed well with the experimental results. Relative errors of ethylene and propylene were not more than 8%.

1. Introduction

Steam cracking of light oil, such as naphtha, mainly produces olefins, such as ethylene and propylene. At present, this is the main way of ethylene production. Cracking, dehydrogenation, ring opening, and coking are main reactions of light-oil steam cracking.

Some methods or models for predicting products of steam cracking have been built. Such as the cracking severity function (CSI) method proposed by Shn et al.,¹ artificial neural network (ANN) model proposed by Niaei et al.,² SPYRO model by the KTI Company,³ and models by Sadrameli et al.⁴ The CSI method is a kind of empirical model. An empirical model calculates quickly and easily but is often poor fitness. Errors are large once the materials change. The model proposed by Sadrameli et al. is a kind of semi-empirical model. Satisfactory results could be obtained with this model. However, a semi-empirical model is based on a summary of a large number of experimental data. The workload of the experiment is large, and applicability of the model is still not wide enough. The ANN model is an ideal model. It can be used to predict product distribution for steam cracking of naphtha. With this model, a good agreement was found between model results and experimental data. However, this mode needs samples to train the neural network; therefore, it still cannot belong to the theoretical model. The SPYRO model is the most successful case of the theoretical model. The model has a

high precision and wide applicability and can calculate the product distribution of the reactor. Therefore, it has been received by industrial applications. However, more than 3000 reaction equations included in the model make the calculation a huge workload.

Although the composition of light oil is relatively simple, steam cracking of light oil still belongs to a complex reaction system. Molecular composition of light oil may be analyzed definitely with an advanced analytical method and instrument, but reaction behaviors of each molecule cannot be described because the number of molecules and reactions is so large. Thus, lumping remains the main way to build a kinetic model of steam cracking. However, the traditional lumping methods can only build a macroscopical kinetic model of steam cracking, which cannot truly reflect the reaction rules of molecules. Its modeling process depends upon the division of the lumping component; therefore, the traditional lumping model cannot predict product distribution accurately when the composition of feedstock changes.

In 1992, Jaffe and Quann^{5,6} proposed a new method to describe composition, reaction, and properties of complex hydrocarbon mixtures called structure-oriented lumping (SOL), which made the knowledge on the petroleum hydrocarbon reaction into a molecular level. SOL described molecular reaction behaviors with structure vectors and reaction rules. It was also a lumping in a sense. However, SOL was based on the idea of the group contribution method. It was a lumping of molecular segments, which was different from traditional lumping. The SOL method laid the foundation for building the molecular kinetic model.

In this work, a kinetic model of light-oil steam cracking has been developed by the SOL method with the help of Materials Studio and Matlab software.

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(1) Wang, S. *Ethylene Process and Technology*; China Petrochemical Press: Beijing, China, 2000.

(2) Niaei, A.; Towfighi, J.; Khataee, A. R.; Rostamizadeh, K. The use of ANN and the mathematical model for prediction of the main product yields in the thermal cracking of naphtha. *Pet. Sci. Technol.* **2007**, *25*, 967–982.

(3) Dente, M.; Ranzi, E.; Goossens, A. G. Detailed prediction of olefin yields from hydrocarbon pyrolysis through a fundamental simulation model (SPYRO). *Comput. Chem. Eng.* **1979**, *3*, 61–75.

(4) Sadrameli, S. M.; Green, A. E. S. Systematics and modeling representations of naphtha thermal cracking for olefin production. *J. Anal. Appl. Pyrolysis* **2005**, *73*, 305–313.

(5) Quann, R. J.; Jaffe, S. B. Structure-oriented lumping: Describing the chemistry of complex hydrocarbon mixtures. *Ind. Eng. Chem. Res.* **1992**, *31*, 2483–2497.

(6) Quann, R. J.; Jaffe, S. B. Building useful models of complex reaction systems in petroleum refining. *Chem. Eng. Sci.* **1996**, *51* (10), 1615–1635.

Table 1. Structure Vectors and C and H Stoichiometric Matrices

| A | A6 | N6 | N5 | R | IH | br | me |
|---|----|----|----|---|----|----|----|
| C | 6 | 6 | 5 | 1 | 0 | 0 | 0 |
| H | 6 | 12 | 10 | 2 | 2 | 0 | 0 |

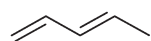
2. Modeling Process

2.1. Feedstock Representation with SOL. Light oil was defined as a hydrocarbon mixture, in which the total carbon number of every molecule was less than 10. To simplify the process of light-oil steam cracking, some limitations were still needed for feedstock molecules: (1) only one or no carbocycle and (2) containing only C and H.

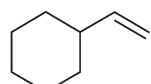
A total of 7 SOL structure vectors were applied to describe molecules. Table 1 showed these 7 structure vectors and their C and H stoichiometric matrix. The carbon content equals $C \times A'$ (transposed matrix of **A**), and the hydrogen content equals $H \times A'$.

The meaning of each vector in **A** is as follows: **A6** refers to benzene; **N6** and **N5** refer to six- and five-membered naphthenic rings, respectively; **R** refers to the total alkyl carbon number; **IH** refers to saturation (except aromatics); **br** refers to the branch point number in a non-ring carbon chain; and **me** refers to the number of side chains in the aromatic or naphthenic rings.

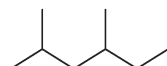
On the basis of these 7 structure vectors, molecules can be described in the form of vector groups, such as follows:



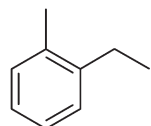
| A6 | N6 | N5 | R | IH | br | me |
|----|----|----|---|----|----|----|
| 0 | 0 | 0 | 5 | -1 | 0 | 0 |



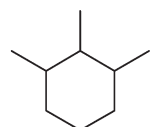
| A6 | N6 | N5 | R | IH | br | me |
|----|----|----|---|----|----|----|
| 0 | 1 | 0 | 2 | -1 | 0 | 0 |



| A6 | N6 | N5 | R | IH | br | me |
|----|----|----|---|----|----|----|
| 0 | 0 | 0 | 8 | 1 | 2 | 0 |



| A6 | N6 | N5 | R | IH | br | me |
|----|----|----|---|----|----|----|
| 1 | 0 | 0 | 3 | 0 | 0 | 1 |



| A6 | N6 | N5 | R | IH | br | me |
|----|----|----|---|----|----|----|
| 0 | 1 | 0 | 3 | 0 | 0 | 3 |

According to the same method, molecules in light oil have been represented as 132 kinds of seed molecules. Table 2 is the number of each category of seed molecules. Generally speaking, any molecule of feedstock, product, and intermediate that satisfied the above limitations could be represented with one kind of seed molecule. For light oil, the content of the molecules that did not satisfy such limitations was small and could be neglected. Therefore, it is feasible to describe light-oil composition with these 132 seed molecules. This is another form of 132 lumping but was different from traditional lumping. Obviously, it is much simpler to treat with such lumping than traditional lumping.

2.2. Reaction Rules. Molecular reaction behaviors of steam cracking are complex; therefore, some reaction rules are needed to make it more ordered and describe the whole process of reactants to products. It has two components: (1) a reactant selection rule to determine if a molecule has the proper structural increments for that reaction and (2) a

product generation rule to generate the product molecule from the structure vector of the reactant.

Reaction rules will change with different processes. Cracking, dehydrogenation, ring opening, and coking are main reactions of light-oil steam cracking. Most of the reactions obey the free-radical mechanism.

Here, 74 reaction rules have been designed to describe light-oil steam-cracking reactions. These reaction rules can be divided into cracking, dehydrogenation, ring opening, cyclization, and coking.

Some typical reaction rules are as follows.

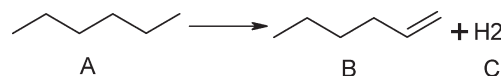
(1) Paraffin cracking (break 2C):



Reactant selection rule: $A6 + N6 + N5 = 0$; $IH = 1$; and $R \geq 3$.

Product generation rule: for B, $R_1 \rightarrow R - 2$ and $IH_1 \rightarrow 0$ and 1; for C, $R_2 \rightarrow 2$ and $IH_2 \rightarrow IH - IH_1$.

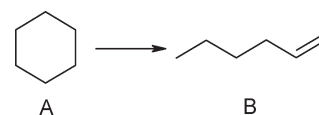
(2) Paraffin dehydrogenation:



Reactant selection rule: $A6 + N6 + N5 = 0$; $IH = 1$; and $R \geq 2$.

Product generation rule: for B, $IH_1 \rightarrow IH - 1$; for C, $IH_2 \rightarrow 1$.

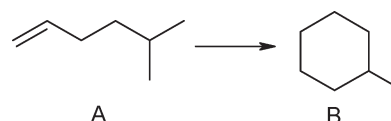
(3) Naphthenic opening (6C):



Reactant selection rule: $N6 = 1$; $A6 + N5 = 0$; and $IH \geq -1$.

Product generation rule: $N6 \rightarrow N6 - 1$; $R \rightarrow R + 6$; and $br \rightarrow me$.

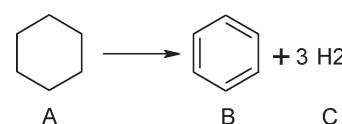
(4) Olefin cyclization:



Reactant selection rule: $A6 + N6 + N5 = 0$; $IH \leq 0$; and $R \geq 6$.

Product generation rule: $N6 \rightarrow N6 + 1$; $R \rightarrow R_1 - 6$; $br \rightarrow \max(0, br_1 - 2)$; $me \rightarrow br_1$.

(5) Naphthenic aromatization:



Reactant selection rule: $N6 = 1$; $A6 + N5 = 0$; $IH = 0$.

Product generation rule: for B, $A6 \rightarrow A6 + 1$, $N6 \rightarrow N6 - 1$, and $IH_1 \rightarrow 0$; for C, $IH_2 \rightarrow 1$.

With these reaction rules, reaction networks can be produced easily. For example, take hexamethylene; a reaction network with hexamethylene is shown in Figure 1.

2.3. Kinetic Differential Equations. All of the reactions of light-oil steam cracking can be treated as first-order irreversible reactions. The reasons are as follows: (1) Cracking

Table 2. Number of Each Category of Seed Molecules

| category | aromatic | 6-cyclane | 6-cyclene | 5-cyclane | 5-cyclene | n-paraffin | i-paraffin | n-olefin | i-olefin | H ₂ |
|----------|----------|-----------|-----------|-----------|-----------|------------|------------|----------|----------|----------------|
| number | 14 | 14 | 14 | 14 | 14 | 10 | 12 | 16 | 23 | 1 |

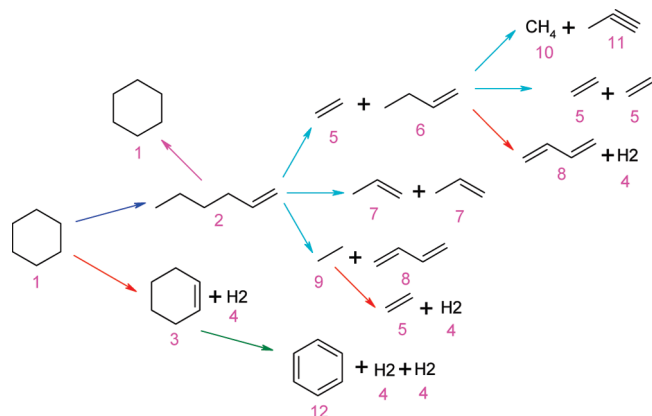


Figure 1. Reaction network for hexamethylene.

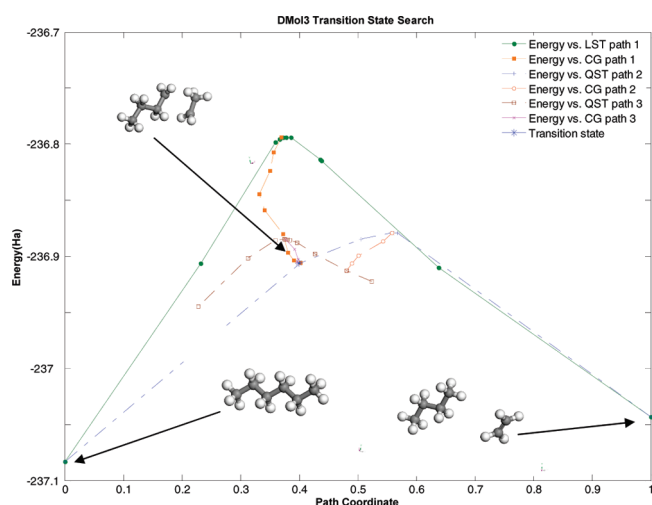


Figure 2. DMol3 transition-state searching.

Table 3. Kinetic Parameters for the Reaction Network in Figure 1

| reaction | <i>E</i> (kcal/mol) | <i>k</i> (s ⁻¹) |
|----------------|---------------------|-----------------------------|
| 1 → 2 | 107.589 | 1.628 |
| 1 → 3 + 4 | 122.969 | 0.841 |
| 2 → 1 | 137.378 | 0.007 |
| 3 → 12 + 4 + 4 | 123.585 | 2.081 |
| 2 → 5 + 6 | 111.981 | 3.289 |
| 2 → 7 + 7 | 98.943 | 4.156 |
| 2 → 9 + 8 | 122.7 | 0.329 |
| 9 → 5 + 4 | 60.421 | 2.562 |
| 6 → 10 + 11 | 110.137 | 2.100 |
| 6 → 5 + 5 | 120.645 | 0.231 |
| 6 → 8 + 4 | 126.476 | 0.626 |

accounting for almost all proportions of steam-cracking reactions is a first-order irreversible reaction in itself.⁷ (2) Ring opening and cyclization are reversible reactions mutually. (3) Although dehydrogenation is a first-order reversible reaction, the cracking reaction rate of unsaturated hydrocarbon from dehydrogenation is much faster than that

(7) Zhou, R. *Cracking Theory and Technology of Petroleum Industry*; Chemical Industry Press: Beijing, China, 1982.

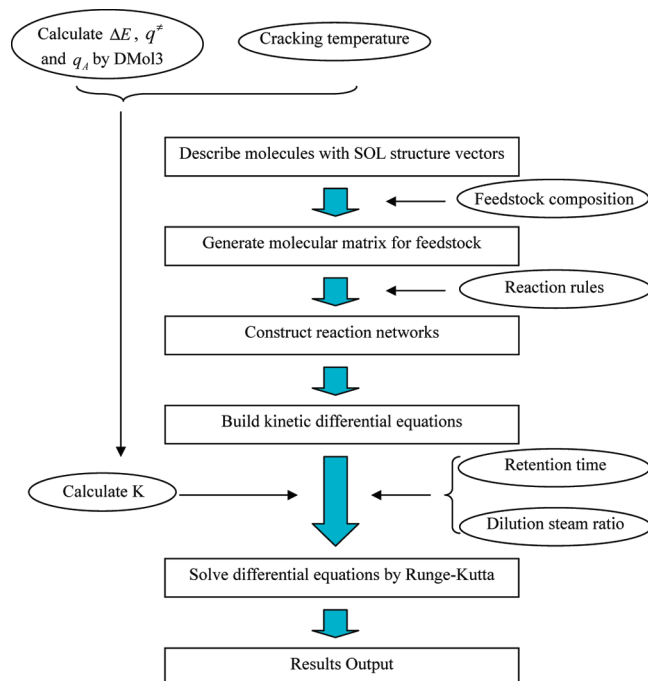
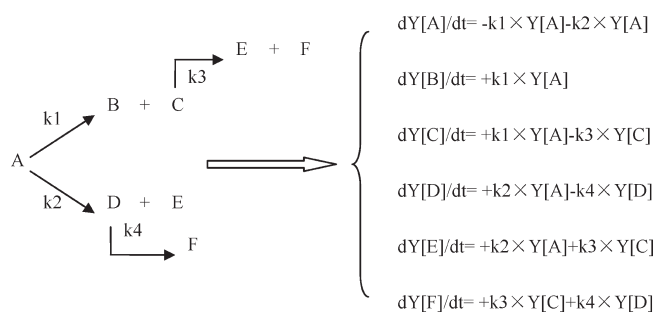


Figure 3. Simulation diagram.

of hydrogenation, and hydrogen in a common circumstance of steam cracking is not enough. (4) Coking is another form of dehydrogenation, which is the same as in reason 3. (5) Few non-first-order reactions can be neglected.

The whole reaction networks from reactants to products are produced by reaction rules. Differential equations for describing kinetic properties of reaction networks can be formulated conveniently because all of the reactions are first-order reactions.

A simple example is as follows:



Although the number of equations will be large with this method, differential equations can be solved with a fourth–fifth-order Runge–Kutta algorithm in Matlab totally because all of the reactions are first-order reactions. The solutions are relative content distributions of these 132 seed molecules with time; thus, product distribution can be predicted.

2.4. Reaction Rate Constant Calculation. Rate constants of every reaction are necessary parameters to solve kinetic differential equations, but the calculation of rate constants has always been one of the difficulties to build a kinetic model.

Table 4. Model Components

| | | | | |
|---------------|---------------|----------------|---------------------------|--------------------|
| pentane (nC5) | heptane (nC7) | decane (nC10) | methylcyclopentane (mcC5) | cyclohexane (cC6) |
| hexane (nC6) | octane (nC8) | i-octane (iC8) | methylcyclohexane (mcC6) | ethylbenzene (aC2) |

Table 5. Composition of Mixtures

| mol | nC5 | nC6 | nC7 | nC8 | nC10 | iC8 | mcC5 | mcC6 | cC6 | aC2 | octene | decene |
|-----|-------|-------|-------|-------|-------|-------|-------|-------|-------|-------|--------|--------|
| 1 | 0.385 | 0.281 | 0.231 | 0.058 | 0.045 | | | | | | | |
| 2 | 0.139 | 0.115 | 0.142 | 0.098 | 0.022 | | 0.100 | 0.152 | 0.232 | | | |
| 3 | 0.120 | 0.070 | 0.070 | 0.102 | 0.032 | 0.262 | 0.098 | 0.126 | 0.120 | | | |
| 4 | 0.122 | 0.100 | 0.063 | 0.070 | 0.038 | 0.116 | 0.097 | 0.089 | 0.145 | | 0.069 | 0.091 |
| 5 | 0.096 | 0.078 | 0.077 | 0.067 | 0.022 | 0.080 | 0.066 | 0.084 | 0.088 | 0.212 | 0.057 | 0.073 |

Table 6. PONA Composition of Naphtha

| Table 1. GC-MS Composition of Naphthas | | | | | | | |
|--|----------------|------------|--------------|--------|-----------|----------|--------|
| hydrocarbon | | n-paraffin | iso-paraffin | olefin | naphthene | aromatic | total |
| SD naphtha | content (wt %) | 30.73 | 35.08 | 0 | 22.78 | 11.41 | 100.00 |
| AQ naphtha | content (wt %) | 27.44 | 32.94 | 0 | 24.73 | 14.89 | 100.00 |

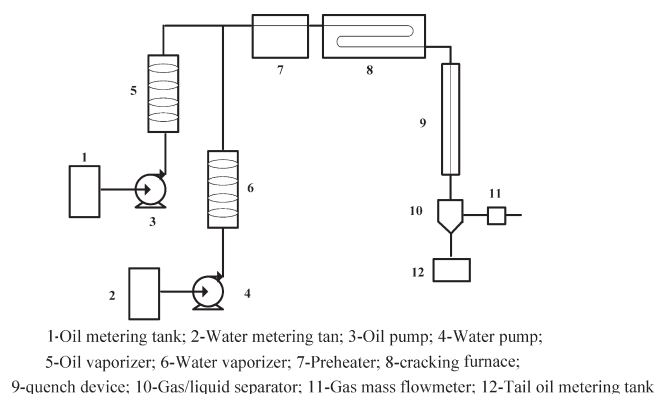


Figure 4. Flow sheet of steam cracking.

For the light-oil steam-cracking process, different researchers obtained different reaction rate constants with different methods.^{8,9}

Equation 1 was applied to calculate the reaction rate constant based on the free-radical mechanism and transition-state theory¹⁰

$$k(T) = \frac{k_B T q^\ddagger}{h q_A} \exp\left(-\frac{\Delta E_0}{k_B T}\right) \quad (1)$$

where k_B represents Boltzmann's constant, T is the temperature, h is Planck's constant, ΔE_0 is the molecular energy difference between the activated transition state and the reactant, q^\ddagger and q_A represent the molecular partition functions of the transition state and reactant, respectively.

$\Delta E/k_B$ in eq 1 can be approximated with $\Delta E/R$,¹¹ where ΔE is the molar energy barrier between the transition state and reactant and R is the molar gas constant. If molecules are described as hard spheres, then the vibration free energy and rotational free energy can be neglected. Thus, ΔE and molecular partition functions q^\ddagger and q_A can be calculated by the DMol3 module of Materials Studio software.

(8) Belohlav, Z.; Zamostny, P.; Herink, T. The kinetic model of thermal cracking for olefins production. *Chem. Eng. Process.* **2003**, *42*, 461–473.

(9) Allara, D. L.; Shaw, R. A compilation of kinetic parameters for the thermal degradation of *n*-alkane molecules. *J. Phys. Chem. Ref. Data* **1980**, *9* (3), 523–559.

(10) Van Speybroeck, V.; Reyniers, M. F.; Marin, G. B.; Waroquier, M. The kinetics of cyclization reactions on polyaromatics from first principles. *ChemPhysChem* **2002**, *3*, 863–870.

(11) Hu, Y. *Physical Chemistry*; Higher Education Press: Beijing, China, 2004.

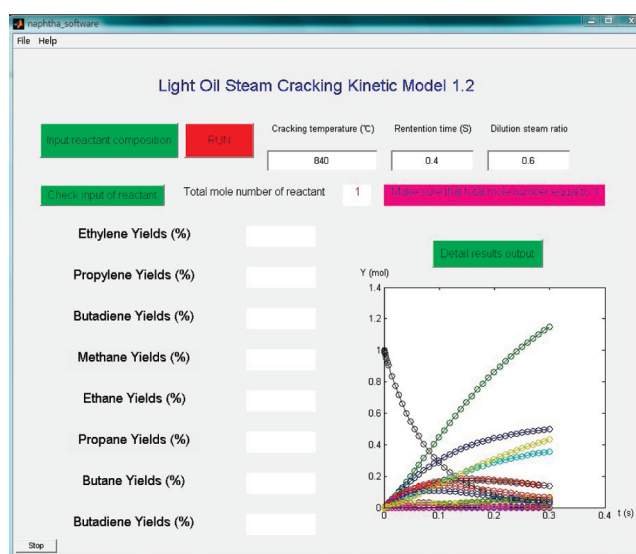


Figure 5. User interface during the calculating process.

Materials Studio is a computer chemistry software from Accelrys Company. DMol3 is an *ab initio* density functional theory (DFT) module based on the first principle of quantum mechanics. It searches the transition state of specific reactions rapidly through combining linear synchronous transition (LST) and quadratic synchronous transition (QST) methods with conjugate gradient (CG) minimization. Then, a series of data related to the transition state, such as ΔE , q^\ddagger , and q_A , can be obtained.

For example, ΔE and the rate constant for each reaction in Figure 1 are shown in Table 3.

For another example, Figure 2 shows the process of transition-state searching of the reaction $C_6H_{14} \rightarrow C_4H_{10} + C_2H_4$.

2.5. Simulation Diagram. The simulation diagram of the model is as follows in Figure 3.

3. Experimental Facility

All of the experimental data of this paper came from the Steam Cracking Facility of the East China University of Science and Technology. Its flow sheet is showed as Figure 4. Raw materials vaporized in an oil vaporizer then went into a preheater to preheat after mixing with dilution steam. Hydrocarbon cracked in the cracking furnace. Cracking gas was cooled off rapidly in a quench device and then was measured and analyzed respectively after gas–liquid separation. Materials and products are analyzed by a gas chromatograph.

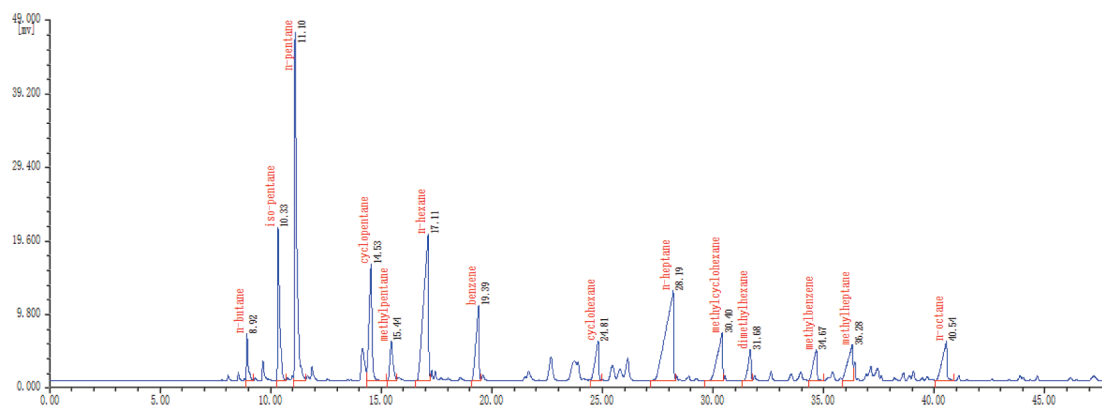


Figure 6. Molecular composition spectrogram of naphtha.

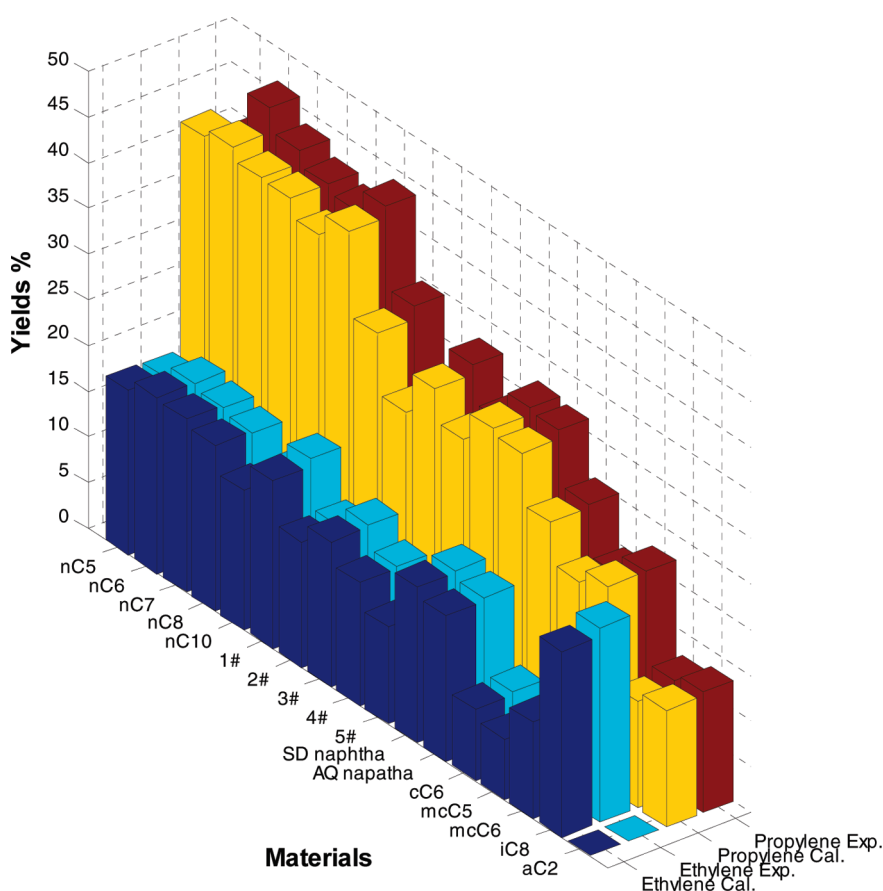


Figure 7. Ethylene and propylene yields for different materials at the same conditions.

4. Simulation Software

Software for simulating the light-oil steam-cracking process has been developed. Seed molecule content distribution with time can be obtained as long as the data of feedstock composition, cracking temperature, retention time, and dilution steam ratio are entered as requested. Figure 5 is the user interface during the calculating process.

5. Results and Discussion

5.1. Materials. A total of 10 kinds of model compounds, 5 kinds of their mixtures, and 2 kinds of naphtha have been used as materials of steam-cracking simulation. Tables 4–6 show model compounds, composition of the mixtures, and

PONA composition of naphtha, respectively. Figure 6 is the molecular composition spectrogram of naphtha.

Ethylene and propylene yields are the most concerned among the products in the light-oil steam-cracking process.

Products yields were calculated from eq 2

$$\text{yield}_{\text{pro}} = \frac{\text{mol}_{\text{pro}} M_{\text{pro}}}{\bar{M} N} \quad (2)$$

where subscript “pro” refers to products to be calculated and mol_{pro} , M_{pro} , \bar{M} , and N refer to the mole number of this product, molecular weight of this product, average molecular weight of materials, and total moles of materials, respectively.

5.2. Model Adaptability for Materials. The typical operating conditions in the industry naphtha steam-cracking

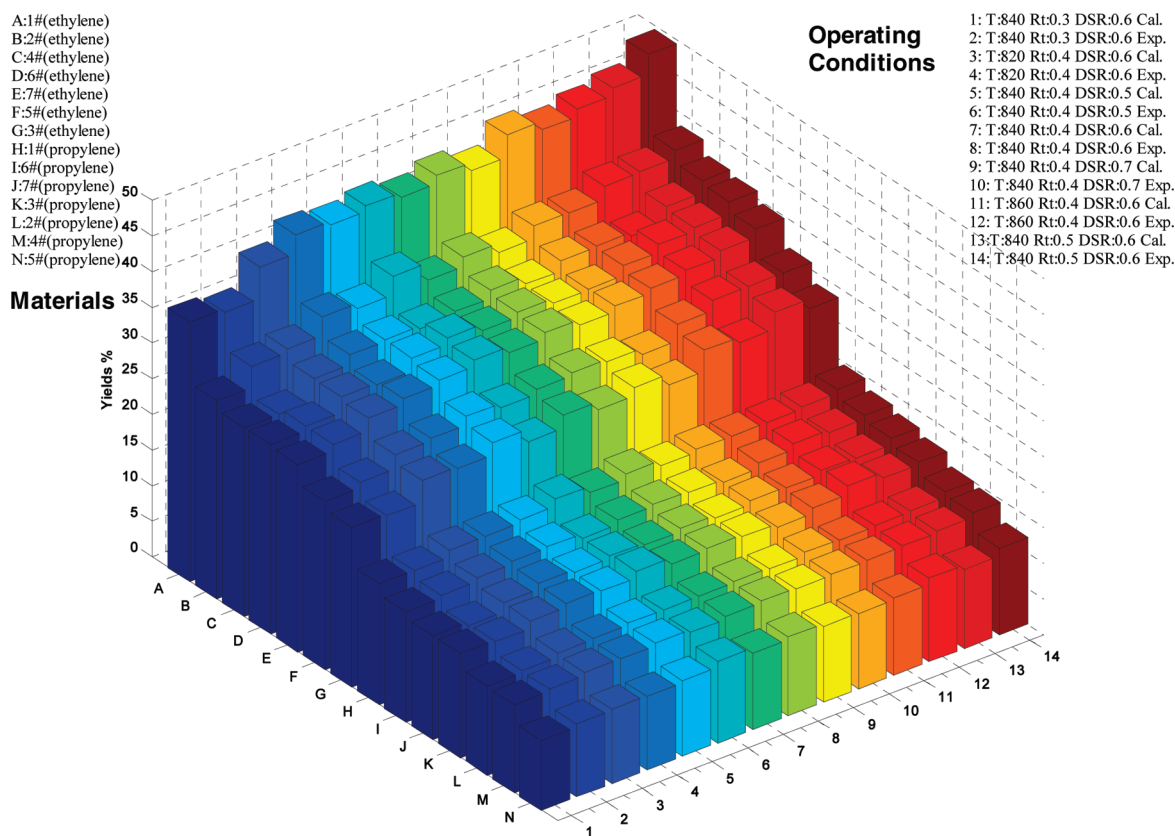


Figure 8. Ethylene and propylene yields for different materials at different conditions.

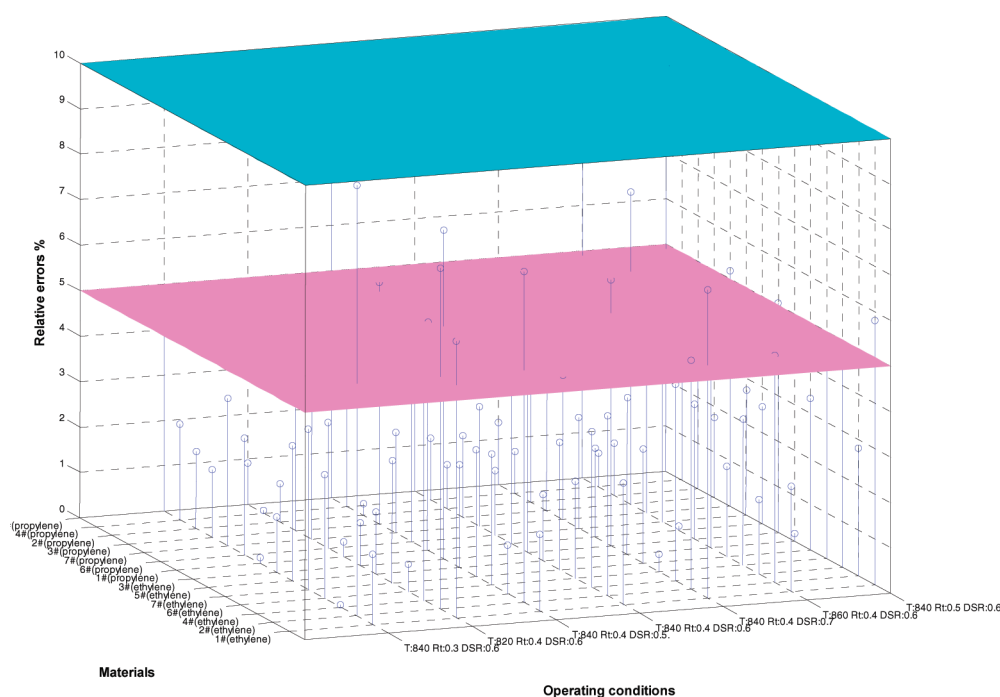


Figure 9. Relative errors of predicted and experimental data.

process are a cracking temperature of 840 °C, retention time of 0.4 s, and dilution steam ratio of 0.6.

Predicted and experimental data of ethylene and propylene yields on steam cracking for the above materials at the typical industry operating conditions are shown in Figure 7.

Figure 7 shows that predicted data of ethylene and propylene yields agree with experimental results well no matter

what the materials are, as long as cracking is at the same conditions. In fact, relative errors of ethylene and propylene yields are less than 5 and 8%, respectively.

That is to say, the model can be applied to the steam-cracking process for different materials.

Reaction rules simplified the real cracking process. Because the model can be applied to different materials, then it

Table 7. Results of Non-main Product Yields

| | materials | temperature | retention time | steam ratio | methane (%) | ethane (%) | butadiene (%) |
|------|--------------|-------------|----------------|-------------|-------------|------------|---------------|
| nC5 | experimental | 840 | 0.4 | 0.6 | 14.65 | 2.30 | 3.75 |
| | calculated | | | | 13.85 | 2.11 | 4.16 |
| cC6 | experimental | 840 | 0.4 | 0.6 | 1.61 | 2.65 | 20.31 |
| | calculated | | | | 1.56 | 2.54 | 19.35 |
| mcC6 | experimental | 840 | 0.4 | 0.6 | 6.87 | 0.81 | 15.70 |
| | calculated | | | | 6.39 | 0.81 | 16.07 |
| 1 | experimental | 840 | 0.4 | 0.6 | 11.59 | 3.08 | 5.44 |
| | calculated | | | | 10.60 | 2.64 | 5.94 |
| 1 | experimental | 840 | 0.5 | 0.6 | 11.70 | 1.89 | 6.11 |
| | calculated | | | | 10.83 | 1.67 | 6.60 |
| 2 | experimental | 840 | 0.4 | 0.5 | 7.38 | 2.45 | 10.67 |
| | calculated | | | | 6.99 | 2.40 | 11.61 |
| 2 | experimental | 860 | 0.4 | 0.6 | 7.77 | 2.16 | 11.34 |
| | calculated | | | | 7.07 | 2.08 | 12.49 |
| 4 | experimental | 840 | 0.5 | 0.6 | 7.31 | 1.30 | 11.87 |
| | calculated | | | | 6.59 | 1.26 | 11.86 |
| 4 | experimental | 840 | 0.3 | 0.6 | 6.61 | 2.82 | 8.03 |
| | calculated | | | | 6.04 | 2.76 | 8.87 |
| AQ | experimental | 840 | 0.3 | 0.6 | 7.41 | 2.57 | 3.62 |
| | calculated | | | | 7.32 | 2.53 | 3.80 |

can be proven that reaction rules for light-oil steam cracking are reasonable and feasible.

5.3. Model Adaptability for Operating Conditions. The principle factors to affect the product distribution of steam cracking are the cracking temperature of the cracking furnace outlet, retention time, and dilution steam ratio. The cracking temperature affects the reaction rate; the retention time affects the cracking severity; and the dilution steam ratio affects the hydrocarbon partial pressure.

Predicted and experimental data of ethylene and propylene yields on steam cracking for the different materials at different operating conditions are as follows in Figure 8.

Relative errors of predicted and experimental data are shown in Figure 9.

From Figure 9, it can be found that most of the relative errors of ethylene and propylene yields are less than 5%, while few relative errors are between 5 and 10%. That is to say, the model can be applied to the steam-cracking process under different conditions.

The influence of principle factors on the results in the model simulation is obviously different from that in a real reaction process. Now that the model can be applied to the steam-cracking process under different conditions, the rationality of assumption and simplification about such an influence in the model simulation can be proven arguably.

5.4. Simulation Results for Non-main Products. Except for ethylene and propylene, the yields of non-main products, such as methane, ethane, and butadiene, can also be predicted by the proposed model. In fact, yields of 132 seed molecules mentioned above can all be predicted.

Some results of non-main products are shown in Table 7.

It shows that the model still has a certain predictive ability for non-main products, although the prediction of non-main products is less precise than that of main products, and it can be proven that the designed reaction rules are reasonable and feasible once again.

The reason why relative errors of ethylene and propylene are less than that of other products is that their amount yields are larger. Although the model can predict yields of all

132 kinds of seed molecules in theory, the deviation of predicted data from experimental data is large for some small content products.

For small content products, deviation is large but can be neglected. For main products, deviation cannot be neglected but is within an acceptable range. It is for this reason that the proposed model can be considered as a reasonable and feasible model.

6. Conclusions

A kinetic model for simulating the light-oil steam-cracking process has been developed via the SOL method and Materials Studio software. The SOL method was used to describe molecules and its reaction behaviors, and Materials Studio software was used to calculate reaction rate constants. The Runge–Kutta method was used to solve simultaneous differential equations. The model can predict distribution yields of all 132 kinds of seed molecules with time. Simulation results indicated that predicted data agree with experimental results well; relative errors of main products, such as ethylene and propylene, are not more than 8% and also a good prediction of non-main products, such as methane. The proposed model could be applied to different steam-cracking processes for different materials under different conditions; therefore, it has a good applicability. The assumption and simplification of the model and the reaction rules for steam cracking of light oil are reasonable. The model is a theoretical model of the molecular level, which does not require any experimental data. Its accuracy, applicability, and workload are all in an acceptable range. It is a good complement for theoretical models and can provide the reference for building other more complex kinetic models.

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