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Lump Kinetic Method in Solving Kinetic Problems and Cracking Reaction Mechanism: A Review

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ABSTRACT

The development of an appropriate kinetic model for cracking reactions is essential for simulation and process optimization. These results are to be potentially used for proper reactor design. The complexities of oil gas inlet combinations have led to an increase in the challenges while defining and depicting kinetics on an intrinsic scale. Hence, complicated chemical reaction circumstances are characterized by combining many possible pathways into more modest groups of comparable chemical substances. In addition, cracking kinetic demonstrations is frequently carried out in lumped forms. This is due to the complex nature of the feedstock, which is known to contain enormous hydrocarbon associated with series and parallel reaction networks. The representation of complicated compounds by consolidating a large chemical component into small amounts of apparent components has been generally utilized in industry to generate a straightforward approach to stoichiometry, thermodynamics, and kinetics. Considering the importance of this lumped method, this study focused on studying the development of a kinetic lump approach to solve kinetic problems and cracking mechanisms.

Keywords: kinetic modeling, cracking mechanism, complex reaction, lumping method

1. Introduction

The kinetics of catalytic cracking reactions are often demonstrated using the lumped method, in which a group of chemical substances with comparative behavior construct a small number of pseudo-species [1]. There are numerous chemical compounds involved in this system, and these reduce the ease to solve reaction rate equations. This problem is potentially resolved by the lumped method, which is estimated to help in the modeling process.

In addition, two essential adaptable strategies are applying this approach, including the primary strategy, characterized by grouping molecules (lumping) according to the boiling point of the group of compounds. This usually consists of feed and products from the cracking process, including diesel, gasoline, gas, and carbonaceous residue.

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The second method is aimed at categorizing items based on the most important chemical derivatives, encompassing paraffin, olefins, naphtha, and aromatics [2].

The first lump model proposed was the 3-lump cracking type for petroleum [3], which was utilized to explain the breaking carbon chain of palm oil [4-5]. This approach, however, has a disadvantage, as the gas and coke, known to have distinct properties, are combined into one lump. These reaction orders depend on the intrinsic abilities of the cracking process. The feed conditions with a mixture of different compounds, known as the primary reactants, suggest a second-order reaction law. Meanwhile, products, assumed to experience elementary and further reactions with limited molecules, adopt the first-order reaction law [3]. This suggested an assumption reported in several studies [4-9].

The 3-lump model was modified and further developed with a more rational approach. According to the 4-lump

model, the coke and gas formation reactions are modeled separately [8], and also the second-order rate law is applied for the oil feed used. The kinetic parameters were evaluated from experimental data and correlated with the feed's characteristics and cracking's operating conditions. This model is also very effective in predicting the coke yield in commercial fixed bed reactors. Gianetto et al. [10] investigated the influence of Y-zeolite crystal size on the gasoline arrangement process.

The 6-lump reaction model is more detailed and is known to solve the vacuum gas fraction oil cracking reaction [7, 11]. This was performed in a microreactor at a reaction temperature of 773 K, and using a commercial catalyst. The rate of decomposition and formation is a component of the substance weight fraction, deactivation function, and reaction rate constant. These properties are consequently used to formulate the reaction rate equation at each step of the 6-lump reaction.

The 6-lump reaction kinetics model is very complicated to be solved because complex reactions are involved, both in terms of material and process. Therefore, specific software is required, and this is achievable using the time-saving function integration method of the Runge-Kutta algorithm with MATLAB software to calculate the parameters [12].

The software has been widely utilized in industries to provide a direct method in the context of the thermodynamics and kinetics of these mixtures. This involves combining an enormous number of substances into a small number of apparent components, to formulate a description of complex mixtures. Furthermore, the cracking process provides a good platform to evaluate various approaches to lumping, because the mixtures involved contain billions of individual compounds, and the technology includes numerous types of chemical reactions and physical separations. Several techniques have been developed specifically in this context and continue to motivate new emerging methods, and are aimed at facilitating more fundamental approaches and achieving a deeper understanding of chemical reactions in complex processes. Considering the significance of lumping, this study focuses on studying the development of kinetic lump methods to solve kinetic problems and cracking mechanisms.

2. Process and Model

The lumping technique is the most widely recognized strategy for building kinetic models. This approach generates dependable outcomes in predicting product distribution and has been generally applied in cracking conventional hydrocarbon oils. Furthermore, the models

are used to carry out kinetic experiments on natural liquid product mixes generated by conducting a catalyzed procedure on vegetable oils [13]. The determination of rate coefficient values through conventional kinetic modeling is limited [14]. This consequence implicates the lumping of similar chemical compounds into pseudo components with specific properties as the best way to manage samples involving complex reactions [15].

2.1. 3-Lump Kinetic Model

According to Ayasse et al. [16], the main product is characterized by a lighter liquid residue or gas, and the 3-lump (**Fig. 1**) is the simplest model capable of explaining this process. This approach has been well studied and reported by Weekman and Nace [3] as well as developed by Wojciechowski [17].

Conceptually, the 3 components were lumped into feed (oil gas), diesel fuel, and light gas (C_1 - C_4 hydrocarbons) with coke. This model leads to the connection between the diesel fuel yield and gas oil conversions. Yared et al. [5] used palm oil as a feed for cracking, wherein aluminosilicate was adopted as a catalyst, and a three-lump model was used. This included the parallel breaking of palm oil into organic liquid, gas, and coke, followed by the parallel cracking of organic liquid into gas and coke. According to the study, there was a constant kinetic increase with an elevation in reaction temperature, specifically in the aspect of organic liquid formation. Furthermore, this model was estimated to be capable of properly representing the experimental data, and the consequent reaction rate equation was formulated based on equations (1-3) as follows [3]:

a. Oil feed cracking reaction

$$r_{Oil} = \frac{dC_{Oil}}{d\tau} = -\phi(k_{12} + k_{13})C_{Oil}^2 \quad (1)$$

b. Gasoline formation reaction

$$r_{gasoline} = \frac{dC_{oil}}{d\tau} = \phi(k_{12}C_{oil}^2 - k_{23}C_{oil}) \quad (2)$$

c. Gas and coke formation reaction

$$r_{gas \text{ and coke}} = \frac{dC_{gas \text{ and coke}}}{d\tau} = \phi(k_{13}C_{oil}^2 + k_{23}C_{oil}) \quad (3)$$

Previous studies adopted 3-lump in the evaluation of product distribution according to the sample boiling points. Callejas and Martínez [18] conducted the hydrocracking of Maya residues and investigated the product yield distribution as well as the kinetics. The experiment was carried out in an Autoclave blended reactor and was heated continuously in an oven by H_2 atmosphere with a pressure of 12.5 MPa and at varied temperatures and weight hourly space velocity. Consequently, the resulting product was divided into

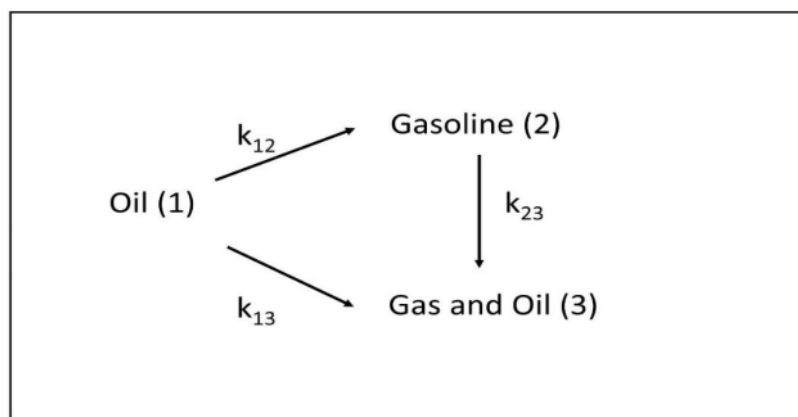


Fig. 1. 3-lump cracking reaction model

various boiling points fractions, and a kinetic model was developed. These included lumped fractions above and below the boiling point of 343 °C (oil) and gas as well. The thermal cracking rate rise to 400 and 415 °C increased the lightest liquid and gaseous fraction yield.

This confirmed the influence of temperature and the decreasing space velocity of the feed mixture on water cracking. The model was evaluated and compared with the experimental data and a decent portrayal was observed. Singh et al. [13] investigated the catalytic cracking of rubber seed oil (RSO) to biogasoline, wherein Cu/ZSM5 was used as a catalyst. According to the study, RSO is primarily transformed into an organic liquid, characterized by a few undesirable coke and gas with a high R^2 value. The most significant rate constant was observed in k_1 at 5.8079. Furthermore, modifications to the 3-lump model have investigated an expanding component of lumps, detachment of coke from light gases, and the proposal of several characteristics relevant in the classification of reaction products into gasoline, LCO, LPG, light gas, and coke.

2.2. 4-Lump Kinetic Model

Cristina [19] observed lump kinetics higher than 3-lump can provide a more correct description of the catalytic cracking process, with better gasoline recovery and lower coke yield. Wu et al. [20] studied the fluid cracking catalytic with a riser and downer reactor. The 4-lump kinetic model was evaluated using a literature review and the result showed satisfactory data fit. These varieties are suggested for distinct heavy oil feedstocks and catalysts. In addition, the four-lump type was constructed to portray crude oil cracking, which produced gasoline, heavy oil, light gas, and coke, where LPG and diesel, for instance, are classified as light gas and crude oil lumps, respectively [21]. Yen et al. [8] designed a simple variant of this model to lessen the difficulties of scaling up techniques.

Fig. 2 shows the cracking model mechanism, where the oil is potentially cracked down into various substances. However, gasoline is more capable of being broken down into gas and coke. The desired reaction product in this process is gasoline, which is possibly used as motor

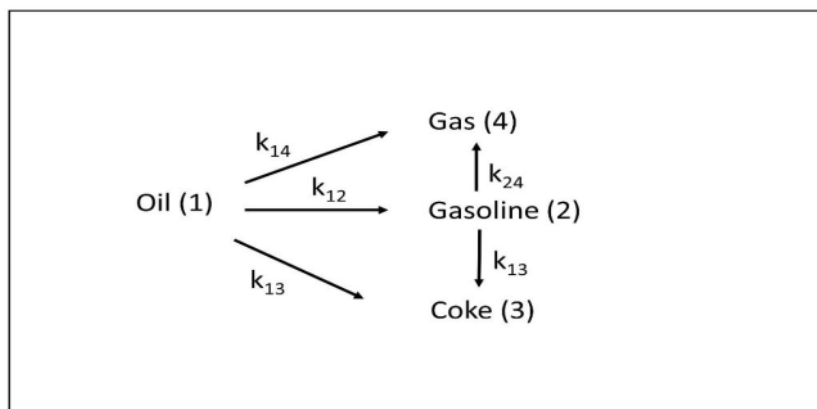


Fig. 2. 4-lump cracking reaction model

fuel. According to Hernández-Barajas et al. [22], a lump with a boiling temperature of n-C₁₂ is expected to be cracked with second-order-kinetics. The first-order conversely applies to lighter lumps. Previous reports showed the five rate constant characteristics of the 4-lump model [23], with the rate equation formulated in equations (4-7) as follows [8]:

a. Oil decrease reaction rate

$$r_{\text{Oil}} = \frac{dC_{\text{Oil}}}{dt} = -\phi(k_{12} + k_{13} + k_{14})C_{\text{Oil}}^2 \quad (4)$$

b. Gasoline formation reaction rate

$$r_{\text{gasoline}} = \frac{dC_{\text{Oil}}}{dt} = \phi(k_{12}C_{\text{Oil}}^2 - (k_{23} + k_{24})C_{\text{Oil}}) \quad (5)$$

c. Gas formation reaction rate

$$r_{\text{gas}} = \frac{dC_{\text{gas}}}{dt} = \phi(k_{14}C_{\text{Oil}}^2 + k_{24}C_{\text{gasoline}}) \quad (6)$$

d. coke formation reaction rate

$$r_{\text{coke}} = \frac{dC_{\text{coke}}}{dt} = \phi(k_{13}C_{\text{Oil}}^2 + k_{23}C_{\text{gasoline}}) \quad (7)$$

Meier et al. [24] proposed a 4-lump model by HBO, WCO, BG, and LBO stoichiometry, representing chemical lumps of heavy bio-oil, waste cooking oil, biogas, as well as light bio-oil, respectively. Consequently, a regression analysis was performed to develop a kinetic model and an understanding of thermal cracking in biomass-based triglycerides. These operations were performed in a persistent mode and under isothermal conditions. Periyasamy [25] reported a comparative study regarding the high temperature cracking models of used cooking oil through lumped monomolecular kinetics, and the chemical lumps were characterized according to the number of carbon atoms in the hydrocarbon. This study revealed greater dominance in the parallel observed compared to the series reaction, and further cracking was also detected. The regression findings revealed a decent acceptance between the predicted and observed values. Schubert et al. [26] utilized a 4-lump model with six reactions to portray the cracking process during the co-pyrolysis of HPR and LDPE, assuming the reactions were monomolecular, irreversible, and first-order. Also, this approach is grouped based on boiling point ranges. The study demonstrates the potential for 4-lump models to reduce difficulties in modeling by considerably reducing the number of components and reactions contrasted with general simulation. Hence, a remarkably reduced handling power is observed. Sadighi et al. [27] employed this model with vacuum gas oil (VGO), and the component of the blended distillate and naphtha including kerosene and diesel, as well as light and heavy naphtha. These samples used as a hydrocracking feed

were assumed to adsorb hydrogen while breaking down into lighter molecules. The amount utilized was more accurately predicted compared to the value calculated from the experimental data. There was also further investigation into the modified four-lump model, comprising unconverted gasoil, mixed naphtha, and light gas [22].

2.3 5-Lump Kinetic Model

A five lump kinetic model was developed to illustrate the catalytic cracking of fuel oil. Fig. 3 shows the specific application with gas oil, dry gas, petrol, LPG, and coke, and seven kinetic constants were identified, including for the deactivation of catalysts [28]. Guerra et al. [29] investigated the reaction characteristics with three types of raw petroleum oil, including medium, improved heavy crude, enhanced variant, and those diluted with bitumen at high temperature. The 5-lump model was initially illustrated using 10 different reaction pathways.

According to Ancheyta-Juárez [28], the primary advantage is the ability to foresee coke production. This product contributes to the temperature needed to endothermically heat and decomposes the raw material, including liquified petroleum gas, hydrocarbons, and dry gases. Consequently, there is a higher possibility to predict the outcome, irrespective of other lumps. The rate equation of the 5-lump model is formulated in equations (8-13) as follows:

a. Oil

$$(r_1) = -(k_1 + k_2 + k_3 + k_4)y_1^2\phi \quad (8)$$

b. Gasoline

$$(r_2) = (k_1y_1^2 + k_5y_2 - k_6y_2)\phi \quad (9)$$

c. Gas LP

$$(r_3) = (k_2y_1^2 + k_5y_2 - k_7y_3)\phi \quad (10)$$

d. Dry gas

$$(r_4) = (k_3y_1^2 + k_6y_2 - k_7y_3)\phi \quad (11)$$

e. Coke

$$(r_5) = (k_4y_1^2)\phi \quad (12)$$

f. Decay function

$$\phi = e^{-k_d t_c} \quad (13)$$

The process of gas oil cracking accompanies a reaction of second-order while diesel fuel and LPG follow first-order. Furthermore, the most reactive molecules from the raw material lumps tend to vanish first, while the leftovers demonstrate a lower kinetic constant. This

outcome is directly proportional to the transformation increments and underlies the reason LPG follows a first-order [30]. A sequential methodology of the 5-lump model has been proposed [31]. In the context of cracking reaction, separation into three models is possible and further characterized by three lumps, respectively. Previous studies also showed the potential for splitting into three other models with four combinations to evaluate the corresponding parameters. The respective parameters are possibly connected to observing the first kinetic model constants. In addition, a portion of the pathway reactions developed is considered equivalent to the first, and the kinetic constants consequently demonstrate similar and comparative values. Sertić-Bionda et al. [32] evolved a five lump kinetic model for gas oil catalytic cracking. The predicted product results were in great concurrence with the experimental data. Hence, this approach was simulated for predictions with fluid materials. Approximately five common oil and gas portions were involved in observing the cracking reactions as well as predicting the conversions and possible fractions. The investigation of distillate fuel oil as separate lumps is proved vital because of the intrinsic inability to adhere to similar principles as other products [15]. The model based on separation is suitable for local limit stock analysis in factories as well as to split liquefied petroleum and dry gas lumps, to match up with commercial applications. Quintana-Solórzano [33] used five lumps, a kinetic model, on bench-scale cracking, and the primary reaction resulted in the quickest conversion of gas oil to gasoline, where about 23 % of the product is capable of undergoing secondary cracking, and over 90 % yield LPG. The coke formed

occurred through a secondary reaction. Al-Sabawi et al. [34] depicted the vacuum catalytic cracking of gas oil using a 5-lump kinetic model, which illustrated the diffusion constraints observed by hydrocarbon species after a link is established with the porous zeolite network. Moreover, the secondary cracking of products to coke is not considered in this model because the kinetic constant for these stages is of a lower magnitude order compared to the initial reaction. The resulting model, which included the impacts of intra-crystallite hydrocarbon molecule transport, proved to be appropriate in determining the overall significance of the species' intrinsic and diffusional kinetics. Zheng et al. [35] used the 5-lump kinetic model in the pyrolysis of vegetable oil asphalt. The reaction was then separated into a raw material lump and four pyrolytic product lumps, including biogas, charcoal, and hydrocarbons. Based on the findings, proper forecasts of the Arrhenius parameters were observed, alongside a strong ability to predict pyrolytic product concentration.

2.4. 6-Lump Kinetic Model

Mu et al. [36] employed a 6-lump model to explain the cracking of residual fuel oil into diverse product distributions, including gas and oil. Another form was also presented, with distinction in the subsequent cracking reaction of LPG and dry gas to coke [37]. This property was based on the premise indicating the possibility of ignoring the additional cracking from one lump to another in an attempt to limit the number of kinetic factors to be considered. In addition, this approach estimates the heat of the reaction and further presents kinetic data [38]. **Fig. 4** shows the cracking mechanism of the 6-lump proposed by Takatsuka [11].

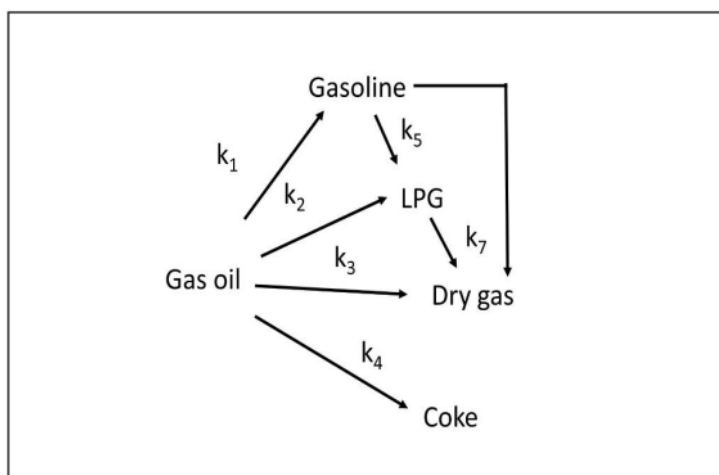


Fig. 3. 5-lump cracking reaction model

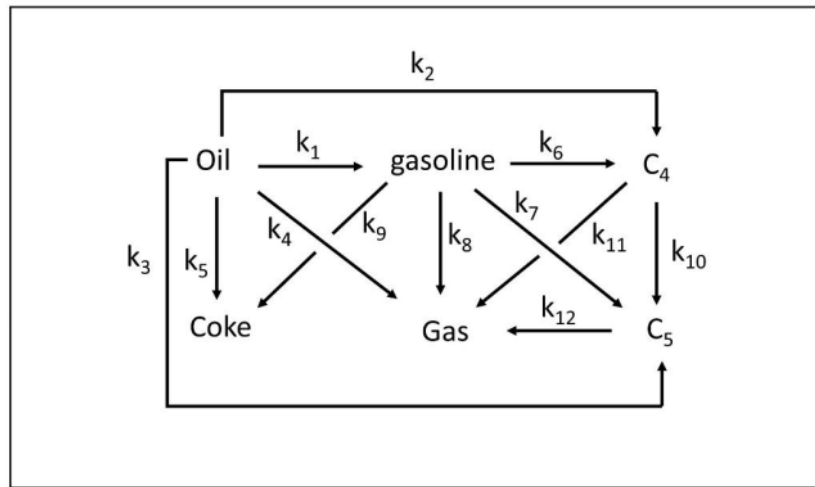


Fig. 4. 6-lump cracking reaction model

The 6-lump model for cracking is formulated in equations (8-13) as follows [11]:

a. Oil decrease reaction rate

$$r_{Oil} = \frac{dC_{Oil}}{dt} = -\phi(k_1 + k_2 + k_3 + k_4 + k_5)C_{Oil}^2 \quad (8)$$

b. Gasoline formation reaction rate

$$r_{gasoline} = \frac{dC_{gasoline}}{dt} = -\phi(k_1 C_{Oil}^2 - (k_6 + k_7 + k_8 + k_9)C_{Oil}) \quad (9)$$

c. C₄ formation reaction rate

$$r_{C4} = \frac{dC_{C4}}{dt} = -\phi(k_2 C_{Oil}^2 + k_6 C_{Oil} - (k_{10} + k_{11})C_{C4}) \quad (10)$$

d. C₅ formation reaction rate

$$r_{C5} = \frac{dC_{C5}}{dt} = -\phi(k_3 C_{Oil}^2 + k_7 C_{gasoline} + k_{10} C_{C4} + k_{12} C_{C5}) \quad (11)$$

e. Gas formation reaction rate

$$r_{gas} = \frac{dC_{gas}}{dt} = \phi(k_4 C_{Oil}^2 + k_8 C_{gasoline} + k_{11} C_{C4} + k_{12} C_{C5}) \quad (12)$$

f. coke formation reaction rate

$$r_{coke} = \frac{dC_{coke}}{dt} = -\phi(k_5 C_{Oil}^2 + k_9 C_{gasoline}) \quad (13)$$

Souza et al. [39] used 6-lump kinetics and a two-dimensional fluid flow to approximate the catalytic cracking of gas oil. This model takes into consideration VGO (unconverted gas oil lump), light cycle oil, petrol, gas fuel, LPG, and coke. Accordingly, the definition identifies gas oil encompasses all lumps, including VGO. Based on a report by Du et al. [40], these kinetic methods have various advantages, including coking and gas cracking as two discrete outcomes, which allow for

yield prediction. Furthermore, the 6-lump model can simultaneously represent the properties of products engaged in the fluid catalytic cracking. Previous studies also showed the potential to function properly in model justification, which is attributed to the apparent rapid simulation and representative concluding data. Sadighi et al. [41] used a variant of this component system, characterized by VGO, diesel, kerosene, heavy and light naphtha as well as gas, while Hernández-Barajas [22] achieved a determination by heavy cycle oil, light cycle oil, light naphtha, heavy naphtha, butane-butylene, and light gas. Despite the high range variations in boiling point, which was dependent on operation, this definition relates to the approximate cut-off boiling point. Xiong et al. [42] simplified the 6-lump kinetic equation by generating various assumptions, where Time-on-flow-based functions and coke-on-catalyst-based functions were the two sorts of descriptions for deactivating FCC catalysts.

2.5. 7-Lump Kinetic Model

Due to the high complexity of the charge stocks in the cracking process, particularly in the aspect of classifying and explaining at the molecular level, efforts were made to group a wide range of chemical mixtures into kinetic species. This was performed to portray the difficult processes. Xu et al. [43] present a 7-lump kinetic model for commercial residual catalytic cracking (RCC) units. The two crude products in the kinetic scheme were handled as byproducts and mixed with vacuum residue and vacuum gas oil as residual fuel oil (RFO) and heavy fuel oil (HFO), respectively. According to the findings of this study, the 7-lump model has the tendency to estimate LPG, dry gas, and

coke production, individually, which is suitable for commercial uses. Also, previous reports showed the appropriateness of offline process simulation and online soft sensor applications, which serve as the foundation for improved process optimization and control. Wang et al. [44] proposed another 7-lump kinetic model, which represents a reaction pathway involving residual vacuum (VR), diesel, gasoline, gas oil, liquified petroleum gas, dry gas, and carbon residue (**Fig. 5**). In addition, a fixed fluidized bed reactor with an isothermal piston flow was utilized. The results revealed a substantially lower secondary cracking rate constant in gas oil than in VR, with an activation energy of 86 to 155 kJ mol⁻¹ and 56 to 100 kJ mol⁻¹, respectively. The model's estimated product outcomes properly matched the experimental data.

The mathematical equation of the 7-lump kinetic model is formulated in equations (14-20) as follows [44]:

$$\frac{dy_1}{dz} = \frac{PMW}{S_{WHRT}} (k_1 + k_2 + k_3 + k_4 + k_5 + k_6) y_1 \quad (14)$$

$$\frac{dy_2}{dz} = \frac{PMW}{S_{WHRT}} [v_{12} k_1 y_1 - (k_7 + k_8 + k_9 + k_{10} + k_{11}) y_2] \quad (15)$$

$$\frac{dy_3}{dz} = \frac{PMW}{S_{WHRT}} (v_{13} k_2 y_1 + v_{23} k_7 y_2) \quad (16)$$

$$\frac{dy_4}{dz} = \frac{PMW}{S_{WHRT}} (v_{14} k_3 y_1 + v_{24} k_8 y_2) \quad (17)$$

$$\frac{dy_5}{dz} = \frac{PMW}{S_{WHRT}} (v_{15} k_4 y_1 + v_{25} k_9 y_2) \quad (18)$$

$$\frac{dy_6}{dz} = \frac{PMW}{S_{WHRT}} (v_{16} k_5 y_1 + v_{26} k_{10} y_2) \quad (19)$$

$$y_7 = (1 - y_1 MW_1 - y_2 MW_2 - y_3 MW_3 - y_4 MW_4 - y_5 MW_5 - y_6 MW_6) / MW_7 \quad (20)$$

A mass balance was used to calculate the coke's concentration lump, and the raw material or the catalyst properties were not considered. This limits the model's usefulness, despite its significant usage.

Sheng et al. [45] described the asphaltene conversion behavior using a 7-lump kinetic model, where the activation energy was observed between 106.07 and 237.50 kJ mol⁻¹. The asphaltene demonstrated the most predominant reaction, which produces heavy and medium oil, characterized by lower activation energies in contrast with the results from thermal cracking. However, coke and gas generation generated higher activation energy than asphalt thermal cracking. The 7-lump model accurately predicts product outputs assumed to be congruent with experimental evidence. Olafadehan et al. [46] discovered outstanding results following the application in industrial residual search catalytic mediation, which was characterized by a mean

absolute variation of 5% between the simulated and experimental data.

2.6. 8-Lump Kinetic Model

Catalytic cracking is a sophisticated chemical system involving high numbers of molecules and causes complexities in the characterization and description of kinetics at this level. The 8-lump kinetic model has received much attention, as observed in Gao et al. [47], where the catalytic cracking of VR was investigated. This approach includes 20 kinetic constants, with catalyst deactivation, which improves the suitability for an application. **Fig. 6** shows the VR lumps in this study were categorized into three sub-lumps, whereas the reaction products are classified into five components based on the intrinsic carbon quantity and boiling point range. The investigation identified an overlap between the cracking capabilities of alkyl carbon, as well as naphthenic carbon with light oil as the primary product. Simultaneously, aromatic carbon is also considered a significant constituent of coke and crude oil.

Several assumptions are utilized to develop the mathematical model, including (1) the raw material evaporates instantly; (2) plug flow for gas and catalyst as well as spiral scattering in the reactor is neglected; (3) isothermal or adiabatic reactor; and (4) the catalyst deactivation is non-specific. The mathematical equation of the model is shown in equations (21-28) as follows:

$$\frac{dC_1}{dX} = \frac{PMW}{S_{WHRT}} (k_1 + k_2 + k_3 + k_4 + k_5) C_1 \phi \quad (21)$$

$$\frac{dC_2}{dX} = \frac{PMW}{S_{WHRT}} (k_6 + k_7 + k_8 + k_9 + k_{10}) C_2 \phi \quad (22)$$

$$\frac{dC_3}{dX} = \frac{PMW}{S_{WHRT}} (k_{11} + k_{12} + k_{13}) C_3 \phi \quad (23)$$

$$\frac{dC_4}{dX} = \frac{PMW}{S_{WHRT}} [(v_{14} k_1 C_1 + v_{24} k_6 C_2 + v_{34} k_{11} C_3 - (k_{14} + k_{15} + k_{16} + k_{17}) C_4] \phi \quad (24)$$

$$\frac{dC_5}{dX} = \frac{PMW}{S_{WHRT}} [(v_{15} k_5 C_1 + v_{25} k_{10} C_2 + v_{35} k_{13} C_3 - (k_{18} + k_{19} + k_{20}) C_5] \phi \quad (25)$$

$$\frac{dC_6}{dX} = \frac{PMW}{S_{WHRT}} (v_{16} k_2 C_1 + v_{26} k_7 C_2 + v_{46} k_{17} C_4 + v_{56} k_{18} C_5) \phi \quad (26)$$

$$\frac{dC_7}{dX} = \frac{PMW}{S_{WHRT}} (v_{17} k_4 C_1 + v_{27} k_9 C_2 + v_{47} k_{15} C_4 + v_{57} k_{20} C_5) \phi \quad (27)$$

$$C_8 = (1 - C_1 M_1 - C_2 M_2 - C_3 M_3 - C_4 M_4 - C_5 M_5 - C_6 M_6) / M_7 \quad (28)$$

The model proposed by Gao et al. [47] exhibited minor differences between the predicted and experimental data while adopting the 8-lump kinetic model. Jiang [48] utilized this approach to describe catalytic cracking for maximizing the isoparaffin process and propylene yield. It demonstrated the potential to precisely predict the main product fraction with varying raw oil compositions. Therefore, relative inaccuracies in the

primary product yield are minimal and meet industrial application needs. Wang et al. [49] described the incidental reaction of FCC gasoline using the 8-lump model. Based on Sani et al. [50], this method is possibly utilized to explain the catalytic cracking of olefins, where predictions match the experimental results.

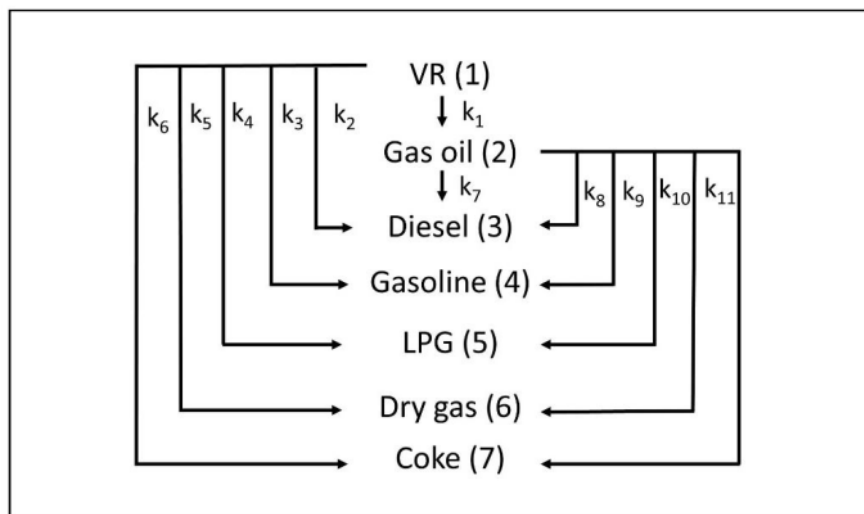


Fig. 5. 7-lump cracking reaction model

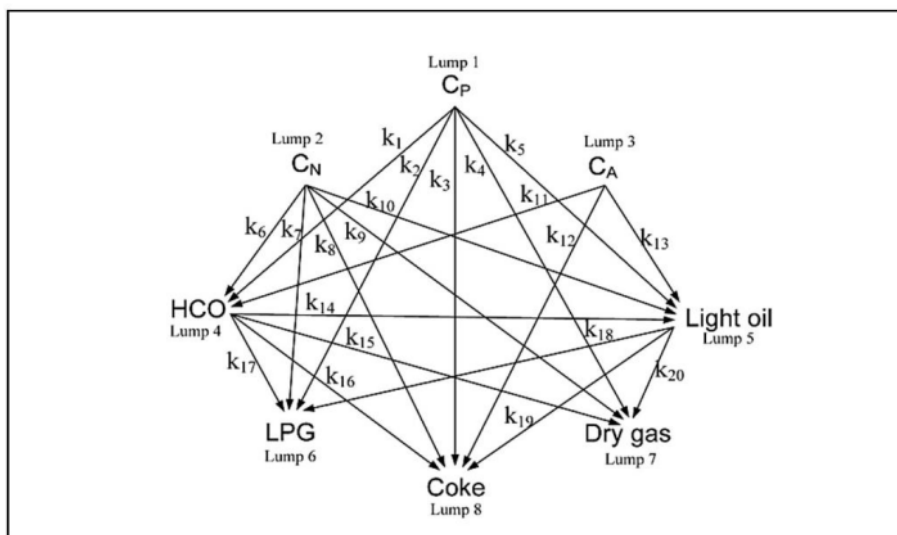


Fig. 6. 8-lump cracking reaction model

2.7. More Than 8-Lump Kinetic

The development of higher-level lump kinetic models has been reported. Zhang et al. [51] studied the cracking accomplishment of six Canadian SCO gas oils and built a nine-lump kinetic model along with three lump feeds for the catalytic pyrolysis of gas oil (**Fig. 7**). These feedstocks provide a considerable impact on product distribution and are expected to be split into lumps, to broaden a range of suitable models. The materials, therefore, have the potential to be separated into three components, including paraffin carbon, naphthenic carbon, and aromatic carbon. In addition, light olefins are one of the products of catalytic pyrolysis, while the by-products include some low molecular weight substances. Studies also showed the occurrence of 24 rate constants as well as catalyst deactivation constants in the 9-lump model. The diesel fuel lump reaction performance is thought to be equivalent to the 7-lump model because the gasoline product exhibits comparable reaction accomplishment. This is considered a reason for the expected findings to be highly similar to the experimental data.

Another work reported the catalytic cracking of VGO utilizing a 9-lump through equilibrium liquid catalytic cracking with a porous catalyst [52]. According to the findings, the resulting products estimated by the model were assumed to be in good concurrence with the experimental data. The Arrhenius model describes the temperature-dependent catalyst deactivation constant, with a frequency factor and activation energy of 2.695

and 65.198 kJ/mol, respectively. You [53] reported the potential for this approach, employing a confined fluidized bed reactor, to estimate yields after exposure to varying reaction temperatures and room rates per hour (WHSV), as well as a catalyst, and temperatures modulated by FCC gasoline. Furthermore, a 10-lump kinetic model was also employed to simulate the cracking reaction. Arandes [54] acclaimed the tendency for an outstanding simulation of the FCC with laboratory-calculated kinetic constants to confirm the correctness of the development model in the simulation program. Du et al. [55] simplified the reaction network in fluid catalytic cracking using a riser reactor, and the results featured the split-up of raw materials and products into ten lumps. This outcome reveals the models' capacity to forecast the major output, and also the intrinsic composition with high accuracy, thus increasing the value in the aspect of propylene yield maximization.

4. Conclusions

The lump kinetics cracking model was designed to be useful in petrochemical processes. These approaches have demonstrated the significance of thoroughly understanding cracking reaction mechanisms in solving important kinetic problems, and also provided a theoretical framework for petrochemical plants. Hence, there is a need to recognize the potential applications in current situations, and also the various computer framework configurations to handle, process, and monitor cracking reactions in real-time.

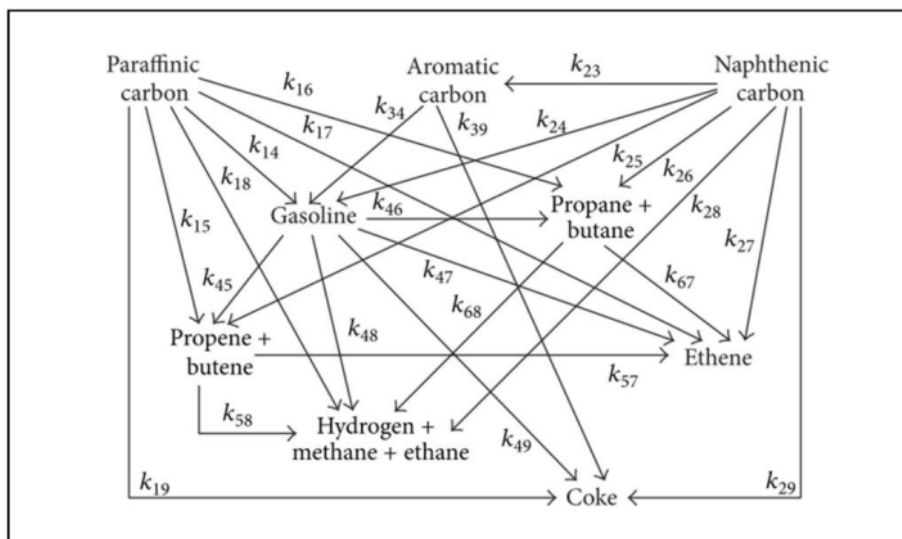


Fig. 7. 9-lump cracking reaction model

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