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Establishment and solution of eight-lump kinetic model for FCC gasoline secondary reaction using particle swarm optimization

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Abstract

An eight-lump kinetic model contained 21 kinetic parameters was proposed to describe the secondary reaction process of fluid catalytic cracking (FCC) gasoline. The model was solved by hybrid particle-swarm optimization (HPSO) which incorporated evolutionary strategies and the simulated annealing method into particle swarm optimization (PSO). A series of experiments were carried out in a riser reactor over an improved Y zeolite catalyst with different temperatures, catalyst to oil ratios and vapor residence times. The product distribution was obtained to estimate the 21 kinetic parameters of model; the calculated results obtained using the HPSO algorithm agreed well with the experimental results.

Keywords: Gasoline secondary reaction; Lumping kinetics; Hybrid particle swarm optimization

1. Introduction

The secondary reactions of fluid catalytic cracking were put forward initially by John and Wojciechowski [1]. Due to the worldwide request for fluid catalytic cracking (FCC) units to produce clean fuel gasoline with low olefins and aromatics, high propylene and *iso*-butylene yields, the effect of secondary reactions on the catalytic cracking process has received more attention. New catalysts for reducing FCC gasoline olefins reported by Raymond et al. [2] and Ye et al. [3] can selectively promote certain secondary reactions like olefins cracking and hydrogen transfer by introducing special active substances into the catalysts. Wang et al. [4] also reported a new FCC processes for reducing gasoline olefin or increasing propylene yields, in which reactors have been improved to provide FCC naphtha secondary reactions with adequate reaction time, space and advantageous conditions.

To design and operate optimally the new processes require improved kinetic models of the FCC gasoline secondary reactions, including the reactive behavior of gasoline olefins, prediction of the distribution of paraffin, olefin, naphthene and aromatic (PONA) composition for gasoline. The lumping method used in the FCC process also can be used to estimate kinetic models of the secondary reaction process of FCC gasoline. It is known that many lump models have been developed for the process optimization of FCC. These models can be categorized into two types. One is composed of the lumps based on the boiling range of the feedstock and its corresponding products, such as the three-lump model by Weekman [5] and Weekman and Nace [6], the four-lump model by Olivera and Biscaia [7], the five-lump models by Corella and Frances [8], Ancheyta-Juárez et al. [9], and the seven-lump model by Sugungun et al. [10]. The other involves the lumps gained on the basis of the molecular structure characteristics of the hydrocarbon group composition in the reaction system, such as the 10-lump model by Gross et al. [11], and the 13-lump model for resid catalytic cracking by Deng et al. [12]. This type of model emphasizes the detailed description

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Nomenclature

$\underline{a_j}$	concentration of jth lump in vapor ($\mathrm{mol}_j\ \mathrm{g}_{\mathrm{vapor}}^{-1}$)	t	time from reaction beginning (s)
$\underline{a}$	vector of concentration of lumps	T	reaction temperature (K)
c_1, c_2	learning factors	t_v	vapor residence time (s); $t_\mathrm{v} = L/u$
E_A	activation energy ($\mathrm{J\ mol^{-1}}$)	u	vapor flow velocity in bed ($\mathrm{m\ s^{-1}}$)
G_V	vapor mass flow rate cross the riser ($\mathrm{g\ m^{-2}\ s^{-1}}$)	x	distance from reactor entrance (m)
$\underline{k_j}$	reaction rate constant of lump j ($\mathrm{m^3\ g_{cat}^{-1}\ s^{-1}}$)	X	relative distance with no dimension, $X = x/L$
K	rate constants matrix	y_j	yield of lump j; y_j^{cal} represents the calculated yield, y_j^{e} is the experimental one
K	constriction factor		
L	effective length of riser reactor (m)	*Greek symbols*	
$\underline{M_j}$	molecular weight of lump j ($\mathrm{g\ mol^{-1}}$)	γ	stoichiometric coefficient
$\overline{MW}$	average molecular weight of vapor mixture ($\mathrm{g\ mol^{-1}}$)	ε	void volume fraction of fluidized bed
n	the lumps number	ρ	vapor density ($\mathrm{g\ m^{-3}}$)
P	reaction pressure (Pa)	ρ_c	catalyst bed density ($\mathrm{g\ m^{-3}}$)
R	gas constant; $R = 8.3143$ ($\mathrm{J\ mol^{-1}\ K^{-1}}$)	ω	inertia weight
r_j	reactive rate of lump j ($\mathrm{mol\ m^{-3}\ s^{-1}}$)	$\varphi_{\mathrm{c/o}}$	catalyst to oil ratio

of the feedstock. However, these lumping kinetic models neglect the composition of gasoline – the most important FCC product, and fail to account for the peculiarity of the olefin molecules. Consequently, they cannot meet the demand of producing clean gasoline.

In this work, based up on experimental results, an improved eight-lump kinetic model which accounts for the boiling range and molecular structure characteristics to describe the gasoline secondary reaction system is proposed. Here, the secondary reaction system is divided by boiling range into dry gas (DG, H_2 and C_1–C_2), liquefied petroleum gas (LPG, C_3–C_4), clean gasoline (GL, C_5^+ −477 K), light cycle oil (LCO, >477 K) and coke (CK); the feed stocks and product clean gasoline (GL) are divided into paraffin (GP), olefin (GO), naphthene (GN) and aromatic (GA) according to molecular structure characteristics. Furthermore, the components of olefin are considered as a separate lump, which permit the simpler description of the kinetic behavior of the olefins in the secondary reaction process. To solve this model, a new algorithm called hybrid particle swarm optimization (HPSO) is introduced to compute the kinetic parameters for FCC secondary reaction system. It is known that the genetic algorithm (GA) is a search algorithm based on the mechanism of natural selection and genetics. GA can achieve a high precision, but is difficult to converge [13–15]. Particle swarm optimization algorithm (PSO) is a population-based optimization technique developed by Kennedy and Eberhart in 1995 [16,17]. Compared to GA, PSO has no evolution operators such as crossover and mutation, it is easy to implement and has few parameters to adjust. However, PSO can be trapped easily into local optima because the swarm loses diversity as convergence proceeds. Simulated annealing (SA) is a global optimization technique based up on annealing of metals [14,18]; it seeks the global optima using stochastic searching techniques. Theoretically, if the calculation time is long enough, simulated annealing method can be guaranteed with probability 1.0 converge at the optimal value.

In this work, a new algorithm called hybrid particle swarm optimization (HPSO) is introduced by incorporating the GA method and SA algorithm into PSO. Using this new hybrid PSO, the kinetic parameters of the eight-lump kinetic model for the FCC gasoline secondary reaction are successful explored, and the reliability of this model is verified.

2. Development of the kinetic model

2.1. Ideal and non-ideal secondary reactions of FCC gasoline

Two kinds of secondary reactions exist in this system [19]. The first one is the ideal reactions for reducing olefin and increasing propylene, including the cracking reactions in the carbonium ion mechanism, hydrogen transfer reactions, aromatization reactions and isomeration reactions. Another is the non-ideal reactions which produce dry gas, olefin components and coke, decreasing the gasoline yield and the octane number. The non-ideal reactions include thermal-cracking reactions in the free radical mechanism, alkylation and dimerization reactions, condensation reactions, dehydrogenation reactions and coke-make reactions.

Neglecting small quantities of non-hydrocarbon compounds like oxygen, sulfur or nitrogen, the secondary reaction network matrix can be written as Fig. 1. Here, if the element in the matrix is '1', there is a reaction from the i row lump to the j column lump; otherwise, no reaction exists or the reaction is ignored.

The features of the eight-lump kinetic model are:

(1) The boiling range is permits decomposition into more lumps.