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Parameter estimation of methanol transformation into olefins through improved particle swarm optimization with attenuation function

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ABSTRACT

This paper provides two improved mathematical expressions of attenuation function to quantify the effect of water in the process of methanol transformed to olefins on SAPO-34. Comparison between the experimental and predicted data shows that the kinetic models, such as four component lumped kinetic model and six component lumped kinetic model, are fitted well by using the improved attenuation functions. In addition, the effect of the error objective function with different weight factors on parameter estimation has been considered. If the maximum component is 10 times greater than minimum, the real weight of each response is more suitably used in the minimization. Meanwhile, double particle swarm optimization is employed to minimize the error objective function and the calculated values agree well with the experimental data.

Keywords: Kinetic parameter estimation; Attenuation function of water; Model discrimination; Particle swarm optimization; Methanol to olefins; SAPO-34

1. Introduction

The transformation of methanol to olefins (MTO) is a conventional method for the production of ethylene and propylene. This process has some advantages over the current steam cracking of hydrocarbons and paraffin dehydrogenation, owing to the truth that MTO can provide a wider and more flexible range of ethylene to propylene ratio relative to those of traditional processes to meet market demand (Fatourehchi et al., 2011). In recent years, some investigations suggested that the reaction of MTO is dominated by a "hydrocarbon pool" mechanism (Arstad and Kolboe, 2001; Dahl and Kolboe, 1993; Goguen et al., 1998; Svelle et al., 2006). Many kinetic models have been built based on the hydrocarbon pool mechanism where the olefins are formed through reversible reactions with large hydrocarbon species.

The kinetic models can be categorized into two main types. One is lumped model, which is a compromise between simplicity and representation of the reality of the process, such as the eight-lump model by Bos and Tromp (1995), the five-lump model by Gayubo et al. (2000). The other is detailed model which takes into account individual reaction steps. In general, it is time consuming or nearly impossible to find the kinetic expressions of a detailed model. And in most cases the lumped kinetic models are sufficient for design purpose.

An acceptable lumped kinetic model not only has to fit experimental data accurately, but also needs to have a group of clear physical significant parameters. It needs us to define a valid objective function and restrict the parameters in a reasonable interval in the process of parameter estimation. In addition, we always have to quantify the attenuation of water in the reaction medium on kinetic steps. Without considering the effect of water content, it is almost impossible to propose an appropriate kinetic model to fit the experimental data. Consequently, the attenuation function has been widely used by many researchers (Aguayo et al., 2002; Gayubo et al., 2003, 2007, 2011) if there is water formed in the reaction medium.

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Nomenclature

a, a_0, a_1, a_2, a_3, a_4, a_5 constant
c_1, c_2 acceleration coefficients
D the number of parameters of the objective function, is the dimension of the space
E_j, E_W activation energy of j step in the kinetic scheme and parameter in the relationship between K_W constant and temperature, J/mol
F^0_{MeOH} initial flow rate of methanol at the inlet of the reactor, mol h^{-1}
k_j kinetic constant of j step in the kinetic scheme (including the attenuating effect of water content in the reaction medium), mol MeOH/(gcat h)
k'_j kinetic constant of j step in the kinetic scheme, mol MeOH/(gcat h)
K_W, K^*_W parameter that quantifies the resistance to the formation of i component in the corresponding reaction step due to the presence of water in the reaction medium, at temperature T and T^*, respectively
MD, G, O, P oxygenates (methanol + DME), lump of gasoline, lump of olefins, lump of light paraffins
M_i molecular weight of i component, mol g^{-1}
n constant
n^M, n^S the number of the master swarm and the number of the slave swarm
n_{exp}, $n_{c\,exp}$ the number of experimental runs and the number of lumps in the kinetic scheme
$pbest_i$, $gbest$, $gbest^S$ the history optima of i particle, the global optimum and the global optimum of the slave swam
q number of parameters to be optimized
r_j reaction rate equation of j step
R Gas constant, J mol^{-1} K^{-1}
R_i rate of formation of i component, mol MeOH/(gcat h)
T, T^* temperature and reference temperature, K
v_i current velocity of particle i
$v_{i,j}$ stoichiometric coefficient of i component in j step of the kinetic scheme
w, w^M, w^S inertial weight, inertial weight of the master swam and inertial weight of the slave swarm
w_{jl} elements of the inverse of the covariance matrix
W amount of catalyst in g
W/F^0_{MeOH} space time of methanol fed, gcat h/mol
x_i the current position of particle i
X_i weight fraction of component i by mass unit of organic components
X_{ij}, $\hat{X}_{ij}$ experimental and calculated data, respectively, of composition for j lump at i experimental point
$X_{oxygenate}$, $X^{in}_{oxygenate}$ weight fraction of oxygenate and weight fraction of oxygenate in the inlet, by mass unit of organic components
X_W, X_{W0}, X_{Wf} water/organic component mass ratio in the reaction medium, in the feed, and in that formed, respectively
y_i yield of i component in g-formed per 100 g of methanol fed to the reactor

Greek letters
Φ error objective function
σ_i symmetry number of component i

Superscripts
* used to describe a composite single-event rate coefficient, i.e., k^*
$\hat{}$ calculated value
M the master swarm
S the slave swarm
t the current iteration

In this paper, the kinetic equation for oxygenates (methanol and dimethyl ether) to olefins is set out as follow:

$$A \xrightarrow{k} B \tag{1}$$

where A = oxygenates, and B = olefins.

The formation rate of olefins, r, which is formulated as a function of the concentration (expressed on a water-free basis) of the corresponding reactant, is assumed to be first order:

$$r = k' X_A \tag{2}$$

where k' is the kinetic constant in kinetic scheme.

To reduce the correlation between preexponential factors and activation energies, reparameterization has been applied (Agarwal and Brisk, 1985). The reparametrized kinetic constant–temperature relationship is

$$k' = k^* \exp\left[-\frac{E}{R}\left(\frac{1}{T} - \frac{1}{T^*}\right)\right] \tag{3}$$

where k^* is a parameter corresponding to the reference temperature, T^*.

To quantify the effect of water, an attenuation function, $\theta(X_W)$, is introduced:

$$k = k'\,\theta(X_W) \tag{4}$$

where k is kinetic constant in the kinetic scheme (including the attenuating effect of water content in the reaction medium).

Two mathematical expressions have been proposed for $\theta(X_W)$ function (Gayubo et al., 2000, 2010):

$$\theta(X_W) = \frac{1}{1 + k_W X_W} \tag{5}$$

$$\theta(X_W) = \exp(-k_W X_W) \tag{6}$$

The constant k_W quantifies the attenuating effect of water. The water content in the reaction medium, X_W, is the summation of the contributions of the water formed, X_{Wf}, and of the water fed, X_{W0}.

Sanchez (1997) used Eq. (5) and defined a following expression to calculate the water formed in the MTO (methanol-to-olefins) process on SAPO-34:

$$X_{Wf} = 0.566 - 0.280X_A + 0.247X_A^2 - 0.311X_A^3 \tag{7}$$

Fig. 1 shows X_{Wf} grows linearly as oxygenate content X_A decreases.

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