Gravitational Search Algorithm for Determining the Optimal Kinetic Parameters of Propane Pre-reforming Reaction

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Introduction

Many metaheuristics algorithms have been successfully applied to solve a wide range of optimization problems. Currently metaheuristic methods are successfully used to solve many problems of engineering optimization, such as multi-robot path planning, un-manned aerial vehicles navigation, the opinion leader detection in online social network, the identification of influential users in social network; the deployment of unmanned aerial vehicles, the data collection system of Internet of Things, the localization in wireless sensor network localization. In this article, we will consider the application of a metaheuristic algorithm, namely, the gravitational search algorithm (GSA), to solve the inverse problem of chemical kinetics in application to heterogeneous catalysis. In recent years, some metaheuristic optimization algorithms, such as Particle Swarm Optimization, Genetic Algorithms, have been applied to solve chemical kinetics problems. However, there is still no persistent conclusion to select a certain algorithm to solve inverse problems of chemical kinetics.

This research is aimed at investigating the effectiveness of metaheuristic algorithms in solving inverse kinetic problems. This work is devoted to the implementation of a gravitational search algorithm for finding the kinetic parameters of an important industrial chemical process. GSA is one of the powerful metaheuristic algorithms currently available that is utilized to solve numerous applications of optimization problems. Furthermore, researchers have proposed a large diversity of methods to improve GSA, such as using enhanced operators, hybridization of GSA with other heuristic algorithms, and parameter adaptation and control schemes for GSA. Despite the fact that GSA appeared recently, it is already widely used. The literature search showed that there is no work on applying the gravitational search algorithm to chemical kinetics problems now, which indicates the relevance of the research.

References

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Mathematical Model

The process under study is propane pre-reforming into methane-rich gas over Ni catalyst, which is an industrially important chemical process [1]. Pre-reforming of propane was studied over industrial nickel-chromium catalyst at pressure of 1 and 5 bar, low steam to carbon molar ratio of 1, in the temperature range of 220-380 ^{0}C and at flow rates of 4000 and 12000 h-1. The experimental data on propane pre-reforming was acquired from our previous work [2]. The reaction scheme consists of two reactions: propane steam conversion and CO2 methanation [3]:

$$C_3H_8 + 6H_2O \rightarrow 10H_2 + 3CO_2$$

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$
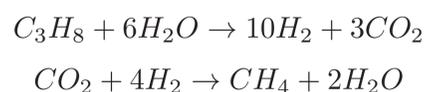
The reaction rates are expressed according to the Langmuir-Hinshelwood model:

$$W_{ref} = \frac{k_{ref} \cdot \exp\left(-\dfrac{E_{ref}}{RT}\right) \cdot C_{C3H8}}{(1 + B \cdot C_{C3H8})^m};$$

$$W_{met} = k_{ref} \cdot \exp\left(-\frac{E_{met}}{RT}\right) \cdot C_{H2} \cdot$$
$$\cdot \left[1 - \frac{P_{CH4}P_{H2O}^2}{K_{eq}P_{CO2}P_{H2}^4}\right];$$

where W_{ref} and W_{met} are the reaction rates; E_{ref} and E_{met} are the observed activation energies, J/mol; k_{ref}^0 and k_{met}^0 are the pre–exponential multipliers; B is the constant parameter, T is the temperature, K; R is the universal gas constant, J(K·mol). The "ref"and "met"indexes refer to pre-reforming and methanation reactions, respectively. C_{C3H8} and C_{H2} are concentrations of propane and hydrogen, mol/m^3; m is order of the denominator, which varied from 0 to 2; K_{eq} is the equilibrium constant of CO_2 methanation; P_{CH4}, P_{H2O}, P_{CO2}, P_{H2} are partial pressures of the corresponding substances, bar. The mathematical model is a system of equations of material balance:

$$\begin{cases} G\dfrac{dy_i}{dl} = \left(\nu_i^{ref}W_{ref} + \nu_i^{met}W_{met}\right)m_i, \\ 0 \leq l \leq, i \in \{C_3H_8, CH_4, H_2O, H_2, CO_2\}, \\ l = 0, y_i = y_{i0}, \end{cases}$$
$$(1)$$

where G is a mass flow of the mixture, kg/(m^2· sec); y_i is a mass fraction of the i-th component; ν_i is a stoichiometric coefficient of the i-th component; m_i is a molar mass of the i-th component, kg/mol; l is coordinate along the catalytic layer, m; L is a length of the catalytic layer, m. The length of the catalytic layer is 0.008 m. The mathematical model of chemical kinetics problems is a system of differential equations that describes the variations in substance concentrations over time according to the rates of reaction stages. The system of differential equations is a Cauchy problem containing the initial data. The numerical solving of such a system of equations is a direct problem of chemical kinetics.

Numerical Experiments

As a result of solving the inverse problem of chemical kinetics by the parallel global search method, the kinetic parameters of the propane pre-reforming process on a Ni catalyst were calculated. To interpret the results obtained, the solution of the direct problem of chemical kinetics was carried out, namely, the concentrations of the reaction components were calculated and compared with the experimental data. Fig. 2 shows a comparison of the calculated concentrations with the experimental ones under different conditions: (a) GHSV=4000 h^{-1}, (b) GHSV=12000 h^{-1}. The results of the calculations are qualitatively consistent with the experiment.

Systems of ordinary differential equations (ODES) describing chemical processes are often stiff due to the presence of fast-flowing and slow-flowing reactions. Therefore, the RADAU-IIA method was chosen as a method for solving the ODE system, which is suitable for solving stiff ODE systems.

The solution of the system of ordinary differential equations is a vector of the calculated concentrations of the reaction components, which are then compared with the experimental data. Determining the kinetic parameters of reaction stages by comparing calculated values of substance concentrations and experimental results is an inverse problem of chemical kinetics.
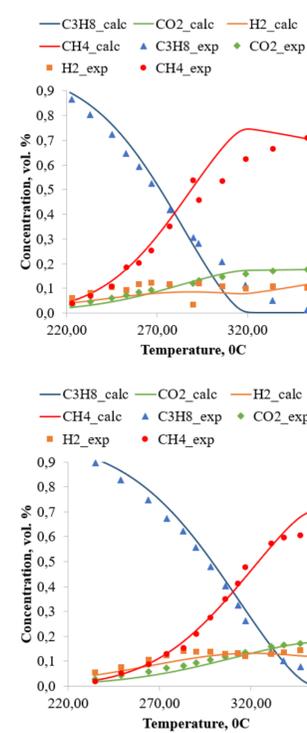
Results

(a)

(b)

Fig. 2. Temperature dependences of the output concentrations of propane C3H8, methane CH4, hydrogen H2 and CO2 in the process of propane pre-reforming. Experimental conditions: (a) GHSV = 4000 h^{-1}, (b) GHSV = 12000 h^{-1}, 1 bar pressure. Points are experimental concentrations ("exp"-index), lines are simulated concentrations ("calc"-index).