A real coded genetic algorithm for the optimisation of reaction rate parameters for chemical kinetic modelling in a perfectly stirred reactor

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Abstract

In this study we develop a real coded genetic algorithm for the determination of the chemical reaction rates parameters (*A*'s, *b*'s and *E*'s in the Arrhenius expression) for the hydrogen combustion in a perfectly stirred reactor (PSR). The algorithm is tested on a hydrogen/air mixture but it can be applied for other, more complex hydrocarbon fuels.

1 GENERAL FORMATTING INSTRUCTIONS

The chemistry of combustion may be modelled using a system of chemical reactions for which the rates of each reaction are known. The net chemical production rate of each species results from a competition between all the chemical reactions involving that species. We assume that each reaction proceeds according to the law of mass action and the forward rate coefficients are in modified Arrhenius form rate:

$$k_{fi} = A_i T^{b_i} \exp\left(-\frac{E_i}{RT}\right) \qquad (1)$$

for $i = 1,\ldots,N_R$, where T is the temperature, $R = 1.9860$ cal mol^{-1} K^{-1} is the universal gas constant and there are N_R competing reactions occurring simultaneously. The rate equation (1) contains the three parameters A_i, b_i and E_i for the i^{th} reaction. Databases that give measurements of reaction rate parameters, (*A*'s, *b*'s and *E*'s in the Arrhenius expression) for various reactions are commercially available, but a large variation in the reaction rates is generally observed. It is the possibility of the determination of these parameters for each reaction, based upon the outlet species mole fractions alone, which is investigated in this study, using a real coded genetic algorithm.

An genetic algorithm optimisation procedure is set up in an attempt to recover the species profiles (to within any experimental uncertainty) resulting from numerous sets of operating conditions by calculating new reaction rate parameters that lie between predefined boundaries. The inversion process aims to determine the unknown reaction rate parameters $((A_i, b_i, E_i), i=1,\ldots,N_R)$ by searching for the set of reaction rates parameters that gives the best fit to a set of given data. If data is measured for N_S different sets of reactor conditions, and all the K species are measured for every reactor condition, then the data will consist of a set of KN_S species concentration measurements and we look for the set of reaction rate parameters that gives the best fit to these measurements. This is done by looking for the maximum of the function

$$f((A_i, b_i, E_i)_{i=1,N_R}) = \left\{10^{-8} + \sum_{j=1}^{N_S}\sum_{k=1}^{K}\left(Y_{jk}^{calc} - Y_{jk}^{meas}\right)^2\right\}^{-1}$$

where Y_{jk}^{calc} and Y_{jk}^{meas} are the calculated and the measured mole concentrations of the k^{th} species in the j^{th} set of reactor conditions. The real coded genetic algorithm employed is found to be very efficient in constructing new reaction mechanisms.