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DETERMINATION OF THE PARAMETERS OF GLOBAL CHEMICAL KINETICS MECHANISMS USING OPTIMIZATION METHODS

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In the paper, an optimization approach to determining global chemical reaction rate constants is proposed. This method allows to select reaction rate parameters (i.e. activation energy, preexponential factor, etc.) on the basis of experimental data or simulations with detailed reaction mechanisms. Computer program implementing proposed method was developed and the features of the application and operation of the optimization approach were investigated.

Although the optimization method can be applied to any reacting system, in this paper the methane-air combustion is considered. Reaction mechanisms are compared by the laminar burning velocity of the premixed flames and the species concentration profiles of the counterflow diffusion flames. To determine the reaction rate constants of global mechanisms, we use an optimization algorithm, which consists in minimizing the deviation between the chosen flame characteristics obtained using a global mechanism and the reference values of these characteristics. Thus, in the case of one flame characteristic (e.g. laminar burning velocity) the following function is subject to minimization:

$$\mathrm{Err} = \sqrt{\sum_i^n (\mathrm{F_i} - \mathrm{F_{GRI-mech\ 3.0_i}})^2}\,, \qquad (1)$$

Where n is the number of different parameter values at which chosen characteristic was calculated, $\mathrm{F_i}$ and $\mathrm{F_{GRI-mech\ 3.0_i}}$ are the characteristic values for the i–th set of parameters calculated using global and detailed GRI-mech 3.0 [1] mechanisms, respectively.

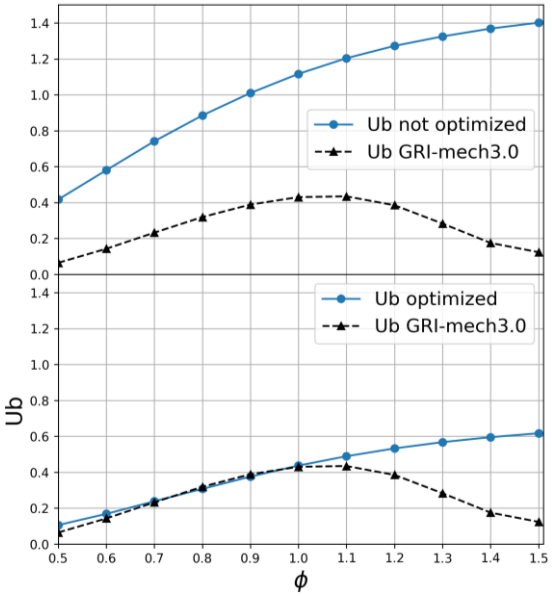

Fig.1. Normal flame velocity before (top) and after (bottom) optimization.

The figure shows a graph of Ub(ϕ), where Ub - laminar burning velocity, ϕ - equivalence ratio. The selected characteristic is calculated with the determined values of the activation energy and the pre-exponential factor in the Arrhenius equation. These parameters are optimized by the algorithm.

It can be concluded that optimization methods are applicable to solve the problems of determination of optimal reaction rate parameters of global mechanisms, providing the best fitting of chosen flame characteristic. Examples of optimization algorithm application for determination of reaction rate constants of one-, two- and four-step mechanisms are presented. The possibility of multi-aim parameters optimization by several characteristics was also investigated and confirmed. It was found that the solution does not have uniqueness, and this fact was confirmed using the brute force method.

REFERENCES

[1] G.P. Smith, D.M. Golden, M. Frenklach, et al. Available at http://www.me.berkeley.edu/gri_mech/.