A Genetic Algorithm-Based Method for the Optimization of Reduced Kinetics Mechanisms

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Abstract

The presented automatic method for the optimization of reaction rate constants of reduced reaction mechanisms is based on a genetic algorithm that aims at finding new reaction rate coefficients in order to minimize the error introduced to the mechanism by the preceding reduction [1]. The prediction ability of the reduced mechanism is assessed against the results from given reference – its full version, another mechanism or experimental measurements, for a homogeneous reactor or laminar-flame simulations under a given set of operating conditions. The deviation between the predictions of the reduced mechanism and its reference is defined by the objective function that is minimized by the genetic algorithm. For the particular problem of the reaction mechanism optimization, the mechanism is encoded as a set of normalized reaction-rate constants (a so-called real-value chromosome) with each individual rate coefficient representing a gene. Usually, the kinetics of each elementary reaction in the mechanisms is defined by the pre-exponential factor A_i, the temperature exponent β_i, and the activation energy $E_{a,i}$. To reduce the dimensionality of the search space, the present method modifies only the forward rate constants of the reactions, until the user-defined criteria within the objective function are met. Since the reaction rate coefficients are mostly determined from experimental measurements or theoretical calculations, a significant uncertainty is associated with these data [2-6] and in many cases the reaction rate modification has to be constrained during the optimization to avoid violating their uncertainty limits. However, collecting and implementing the uncertainty limits for each elementary reaction in the mechanism can require tremendous effort, especially for mechanisms of complex hydrocarbons where many reaction rates and their uncertainties are unknown. To reduce this effort, we introduce a penalty function within the objective function that aims at keeping the reaction-rate constants close to their nominal values. The penalty function approach can be combined with predefined uncertainty bounds for each reaction of the mechanism, where the uncertainty limits are well known and important to maintain. This approach is demonstrated for hydrogen mechanism by Konnov (2008), [7] for which the uncertainty factors of each elementary reaction is listed (Figure 1). Where the physical meaning of chemical data is not required, the penalty function can be relaxed or omitted, enabling a further reduction or optimization towards other targets. This may be necessary for complex CFD where the mechanisms must be significantly simplified and adjusted to the specific range of operating conditions. A reduction of the mechanism during the optimization achieved by adjusting the penalty function accordingly is demonstrated for the reduced version of *tert*-butanol combustion mechanism by Sarathy et al. (2012), [8].

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The optimization method has shown to be robust, flexible, and suitable for a wide range of operating conditions by using multiple criteria simultaneously.

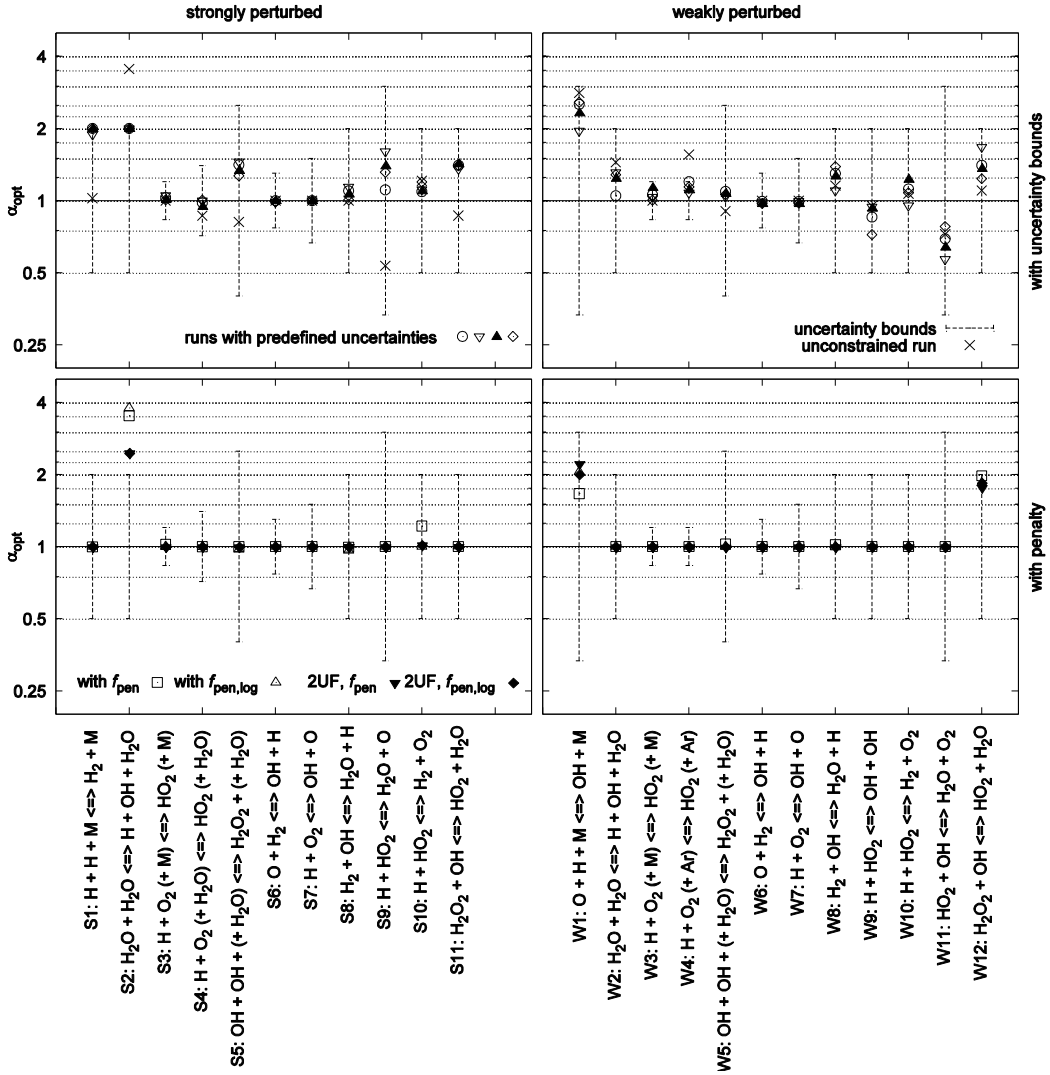

Figure 1- Extent of reaction rate modifications in comparison to their uncertainty bounds for optimization runs performed on two reduced hydrogen mechanisms with different degrees of perturbation.

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