

Efficient tool for optimization of chemical kinetics

As computational power increases, more complex chemical kinetics can be used in the numerical simulation of turbulent reacting flows. However, the increased size of a chemical mechanism also results in an increased number of uncertain parameters, which in turn impacts the predictive nature of numerical simulations. In this framework, the use of optimization techniques becomes crucial to reduce the inherent uncertainty of detailed chemical mechanisms. The focus of this work is to develop an efficient tool for optimizing kinetic schemes, by utilizing the Dakota toolbox for the optimization, and the OpenSMOKE++ framework for the chemical kinetics simulations. This allows the user to specify high fidelity experimental targets from various sources, such as Plug Flow Reactors, Jet Stirred Reactors, Batch Reactors, Ignition Delay Times etc. Thus, by optimizing the kinetic parameters which has the largest impact with respect to the experimental targets, the user can find the optimal combination of these parameters in order to improve the prediction of the kinetic mechanism for these conditions.

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