Bachelor’s / Master’s Thesis

Development of Optimization Strategies for Chemical Kinetic Combustion Models

The chemical kinetics of fuels are of high relevance for modeling of ignition and combustion in energy conversion machinery. Detailed chemical kinetic mechanisms are typically developed based on experimental investigations, quantum-chemical calculations, assumption of similar kinetic behavior in so-called reaction classes, and/or by means of automatic optimization methods. At the same time, CFD simulations with acceptable computational costs typically require reduced mechanisms.

The accuracy of model output at specific conditions of interest greatly depends on how accurately the model parameters are determined. Especially the kinetic rate parameters and the thermochemical parameters often have large uncertainties. Therefore, the output quantities predicted by the model, such as ignition delay times or laminar burning velocities, also have considerable uncertainties. Recent research aims at quantifying these prediction uncertainties and at optimizing the models based on experimental target results.

In this thesis, existing automatic methods for analysis of chemical kinetic models and for optimization of relevant model parameters shall be extended. For instance, kinetic and thermochemical parameters, which have only been optimized separately in the past, can be optimized simultaneously for better model prediction. Depending on the personal interest and knowledge, the focus of the thesis can be adjusted individually. A simultaneous Hiwi employment is possible.

Possible tasks:

- Extension of an optimization framework for kinetic and thermochemical model parameters
- Analysis of the impact of parameter uncertainties on model prediction
- Implementation of adjoint methods for sensitivity analysis

Your prerequisites:

- High motivation & ability to work independently
- Interest in combustion & chemical kinetics
- Interest in programming & simulation
- Preferably TV I exam successfully passed

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