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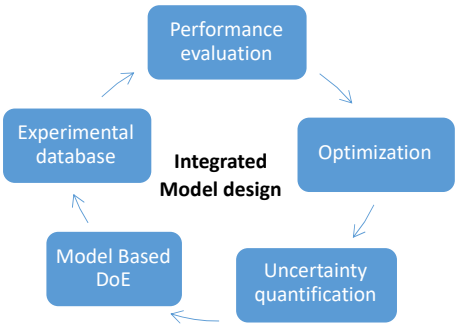
Bachelor- / Masterarbeit
Comprehensive quantitative evaluation and improvement of chemical kinetic models

Within the Cluster of Excellence - “The Fuel Science Center,” our focus is to understand the molecular interactions in fuel combustion and translate that information to practical applications. This is done by means of chemical kinetic models.
To facilitate the development and design of new alternative fuel-based practical applications, accurate chemical kinetic models are needed that can describe the combustion under technically relevant conditions. In this regard, we establish a large experimental database of combustion quantities such as laminar flame speed. We compile all the latest models describing fuel combustion and test them. A quantitative metrics is established to arrive at best-performing model. There is often need to further improve the models and a systematic optimization is performed towards this. The optimized model shows better performance than all other models. This model is used to do design of experiments which can guide experimenters with conditions at which they should perform experiments for model uncertainty minimization. This whole mathematical approach enables a systematic improvement of the current kinetic models. We have already utilized this methodology for ammonia/hydrogen combustion. We plan to apply this to improve NOx prediction mechanisms, which is the hour of the need.

Your Tasks

Extend the methodology for other fuels/mechanisms

- Establish experimental database
- Test recent mechanisms under this method and report the best-performing model
- Further improvement of the model with systematic optimization



Integrated model design approach for developing chemical kinetics models to describe combustion of alternative fuels

Your requirements

- High motivation and independent working style
- Good hold on Mathematics and python-coding

Our offer

- Collaboration in current, highly relevant research projects
- Publication in a high-ranked journal
- Possibility to extend this as a Master thesis

Contact person

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If you have questions, feel free to write to me. If interested, please send a brief resume and grade transcript!