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Bachelor- / Masterarbeit
Fuel structure to combustion to emissions

Within the Cluster of Excellence - “The Fuel Science Center,” we develop a predictive simulation process for the screening of novel bio-hybrid fuel candidates. Beginning from the molecular structure of the fuel, to the combustion and emission predictions.
One missing link in this integrated modeling is fuel molecular structure to chemical mechanism. Chemical mechanism, characterized by species, reactions and their rate constants, describes detailed chemistry of combustion. Typically, the mechanisms are developed individually for each fuel with several quantum chemistry calculations or direct rate measurements. Another possibility is to apply analogy from chemistry of similar known fuels. We have developed an automatic code for doing this systematically. We also complement this with rate constant estimation using neural network model.

Your Tasks

Integration of the mechanism generation methods. Further integration into the integrated QSPR model

- Implementing state-of-the-art rate rules in the existing code
- Test the neural-network framework and integrate it with the above method
- Final integration with the QSPR model

Your requirements

- High motivation and independent working style
- Interest in Coding, Mathematics and Chemistry (optional)

Our offer

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

Contact person

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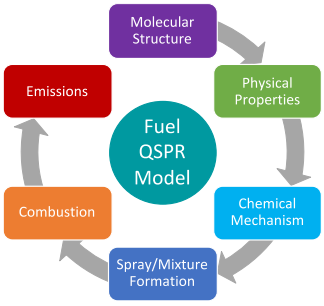
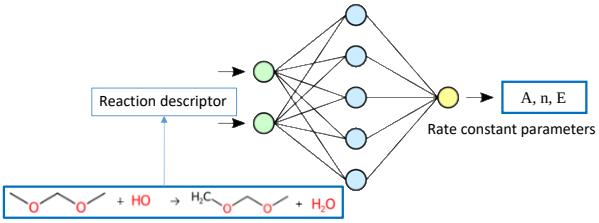
If you have questions, feel free to write to me. If interested, please send a brief resume and grade transcript!



ITV • WSA • IFAS • MBFD • PCFC • VKA

Integrated QSPR model from fuel structure to emissions. Chemical mechanisms is key to describe the chemistry of the system



Neural network model for rate constant estimation. It is trained using extensive database of calculated/measured rate constants