# Bio-hybrid Fuels: From Molecular Structure to Combustion and Emissions

**Topic is suitable for**

- ✓ HiWi Work
- ✓ Bachelor thesis
- ✓ Master thesis

**Field of activity**

Chemical kinetics
Spray combustion modeling

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In the research project conducted within the Cluster of Excellence - "The Fuel Science Center," our focus is on the advancement of a predictive simulation process used for screening new bio-hybrid fuel candidates in terms of emissions. The model utilizes the molecular structure of a fuel as input and generates predictions for spray combustion and emission outcomes. A 1D turbulent spray combustion model, termed 'CARTS', has already been developed at ITV for this purpose. CARTS requires a chemical kinetic model to accurately represent the intricate combustion chemistry involved. Typically, creating such models for individual fuels is a challenging task due to the need for computationally expensive quantum chemistry or empirical measurements for thousands of parameters, making this endeavor impractical. To overcome these challenges, we are planning to explore an innovative framework that incorporates two key ideas:

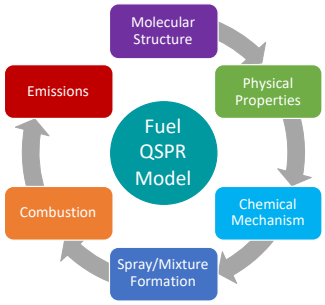


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**Fig. 1. QSPR model**

- Reaction classes: Utilizing known similar fuels to predict potential reaction schemes: By drawing on the knowledge of fuels with similar characteristics, we aim to forecast the likely reaction pathways for the new bio-hybrid fuels under investigation.
- Machine Learning: Applying machine learning techniques to predict rate parameters: To characterize the reactions in the chemical kinetic model, we employ machine learning algorithms. These algorithms learn from available data and generate predictions for the rate parameters associated with the reactions.

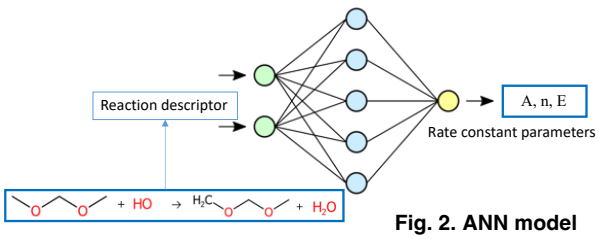


**Fig. 2. ANN model**

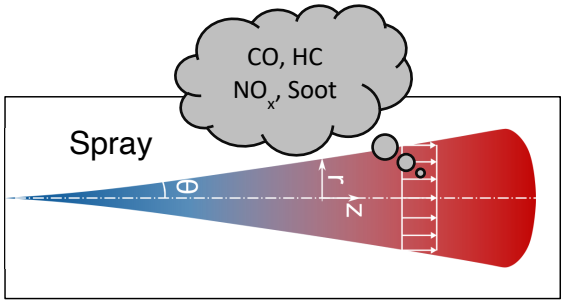


**Fig. 3. CARTS model**

Through the combination of these two approaches, we aim to develop an automatic framework that can generate chemical kinetic models efficiently and effectively, bypassing the need for extensive quantum chemistry computations and significantly reducing the complexity of the modeling process.

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## Tasks

- ◊ Refinement of the existing model based on the above-mentioned key ideas
- ◊ Comprehensive testing of the integrated model for various known fuel
- ◊ Integration of the model with CARTS for spray combustion simulations

## Requirements

- ◊ Strong expertise in coding (preferably Python and Fortran)
- ◊ Fluent in English
- ◊ Ability to work independently
- ◊ Self-motivation and commitment

## Our Offer

- ◊ Highly collaborative and interdisciplinary environment
- ◊ Upto 10 HiWi hours
- ◊ Publication in a high-ranked journal

## References


1. Deshmukh A. Y. et al., A reduced-order model for multiphase simulation of transient inert sprays. International Journal of Multiphase Flows 147 (2022), 103872.
2. Deshmukh A. Y. et al., A reduced-order model for turbulent reactive sprays in compression ignition engines. Combustion and Flame 236 (2022), 111751.
3. Cai L. et al., Auto-ignition of oxymethylene ethers ($OME_n$, n = 2–4) as promising synthetic e-fuels from renewable electricity: shock tube experiments and automatic mechanism generation, Fuel 264 (2020), 116711.