Electrofuel Synthesis for Aviation

Fundamental Investigation of Electrofuel Synthesis by Molecular Dynamics Simulations

S. Rabet[1,2], A. Mecklenfeld[1,2], G. Raabe[1,2],
1. Institute of Thermodynamics, TU Braunschweig.
2. Cluster of Excellence SE²A, Sustainable and Energy-Efficient Aviation, TU Braunschweig, Germany.

In Short

- Detailed investigation to lay the scientific foundation for the production of aviation fuels via electrosynthesis.
- Study structure and dynamics of the reaction system in the currentless and polarizable electrochemical cells.
- Calculate the potential of mean force (PMF) to describes the binding affinity of a solute to the electrode surfaces.

Human-made greenhouse gases are causing considerable changes on Earth's climate that could adversely affect societies and individuals. Among all sources of emission, aviation is one that has great climate impact. [1]
Therefore, it is a global objective to find methods and technologies for significantly reducing the CO_2 footprint of aviation. One way to decrease flight emission is to change the type of energy sources for flight vehicles.
The project C2.1, *Fundamentals of Electrofuel Synthesis for Avation*, is part of the interdisciplinary SE²A cluster of excellence at TU Braunschweig, in which technologies for sustainable and environmentally friendly aviation are studied. The objective of the project C2.1 is to lay the scientific foundation for the production of aviation fuels via electrosynthesis. For this purpose, the molecular dynamics simulation (MD) approach will be utilized to complement the experimental electrochemical and bioelectrochemical research of the projects' partner to develop a knowledge-based toolbox for an energy-efficient aviation fuel synthesis.
All MD simulations for this project will be performed by LAMMPS [2] and GROMACS [3]. Each simulated system consists of two metal electrodes made of promising electrode materials for hydrogenation and hydrodeoxygenation, such as copper, lead and nickel. Moreover, the fluid phase between the two electrodes consists of water and different electrolytes and reactants. The reactants to be studied in the first phase of project comprise furfural, hydroxymethylfurfural (5-HMF) and levulinic acid as educts and valeric acid, 2,5-dimethylfuran, 2-methylfuran as products. In this phase of the project, the investigated electrolyte will be sulfuric acid.
The scheme for one of the electrofuel cell configuration is represented in Figure 1. It consists of copper electrodes on the right and the left side of the simulation box, and water solution with 5-HMF molecules.

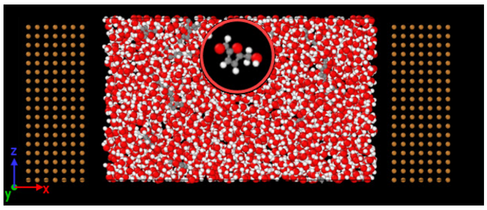

***Figure 1:** Setup configuration of an electrochemical cell containing 5-HMF and water with Cu electrodes.*

The electrode-electrolyte interactions will be investigated for the impact of electrode materials and structures, and of the electrolyte composition on the electrocatalytic properties and reaction mechanisms in currentless and polarizable electrochemical cells. The molecular arrangements and adsorption trends of educts and products at different electrode surfaces will be analysed by radial distribution functions (RDFs), by determining the reorientational correlation times of their molecular vectors and by determining their potential of mean force (PMF) as function of their distance from the electrode surface. A depiction of a PMF curve for a 5-HMF molecule in water solution near copper electrode is given in Figure 2.

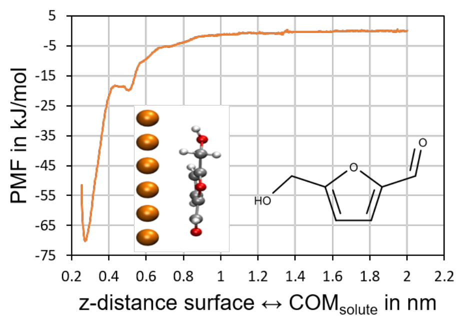

***Figure 2:** PMF curve for a 5-HMF molecule and copper electrode with regards to reaction coordinate z*

Furthermore, to get an insight into the role of the electrolyte, the local solvation structure around the moieties of the reaction system will be analysed by using RDFs and by determining the coordination

numbers. The dynamic properties of the different moieties will be studied by determining their diffusion coefficients both in the adsorbed layers at the electrode and in the bulk phase.
All in all, various MD methods will be used to understand the structural and dynamic behaviors of the systems. The results from the MD studies will be related to the experiments in order to identify relevant interaction patterns and molecular determinants for an optimized, tailor-made electrochemical fuel synthesis.

WWW

https://www.tu-braunschweig.de/se2a

More Information

[1] Jardine, Christian N. "Calculating the environmental impact of aviation emissions." Envirомental Change Institute, Oxford University Centre for Enviroment, 2005.

[2] Plimpton, Steve. Fast parallel algorithms for short-range molecular dynamics. No. SAND-91-1144. Sandia National Labs., Albuquerque, NM (United States), 1993. doi:10.2172/10176421

[3] Abraham, Mark James, et al. "GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers." SoftwareX 1 (2015): 19-25. doi:10.1016/j.softx.2015.06.001

Project Partners

Prof. Dr. rer nat. habil Uwe Schroeder, Institute of Environmental and Sustainable Chemistry, TU Braunschweig.
Prof. Dr.-Ing. habil Antje Spiess, Institute of Biochemical Engineering, TU Braunschweig

Funding

Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy- EXC 2163/1, Sustainable and Energy Efficient Aviation, Project-ID 390881007.