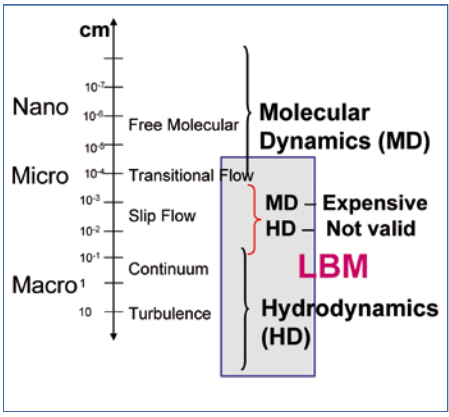
CEMTEC

Computational Engineering of Multi-Scale Transport in Small-Scale Surface Based Energy Conversion

Scope of project

The scope of the present work is to develop a numerical tool for the simulation of multicomponent reacting flows in porous media with specific applications in solid oxide fuel cells (SOFC) and microreactors for portable power generation. The collaboration among different partners will provide to the numerical groups the data needed for the implementation and validation of novel accurate models. Moreover, once the models are implemented and are ready to simulate realistic systems, the experimental groups will benefit from the calculations in optimizing their experimental setups and eventually in building a micro-fuel cell prototype.



A schematic diagram indicating the domain of validity of the Lattice Boltzmann Method for various system sizes.

Goals and activities of the project

- LAV-ETHZ: A new, complete and systematic array of Lattice Boltzmann models have been derived implemented and tested with the specific focus on compressible flow simulation and simulation of micro-flows beyond continuum physics.
- PSI: In a close collaboration with LAV-ETHZ, Lattice Boltzmann models for simulation of multicomponent mixtures were constructed, implemented and extended to include surface-based chemical reactions.
- LTNT-ETHZ: A study of reforming efficiency of Rhodium nanoparticles has been completed based on the experimental investigation of a reacting multicomponent flow in porous micro reactors. The acquired data about kinetics of the reactions will serve as a basis for the validation of computational models of SOFC porous anodes. A macroscopic model of SOFC anodes with internal reforming of water steam/methane mixture has been developed utilizing a Computational Fluid Dynamics (CFD) software package.
- EPFL: A new method to desensitize Ni-cermet SOFC anodes, molten carbonate fuel cell anodes and fuel processing catalysts against sulphur and manufacture thereof was invented and developed.
- Empa: Chemical speciation of sulfur on a set of SOFC pristine and operated anodes was carried out using S(1s) x-ray absorption spectroscopy.

Main scientific results of workgroups

LAV-ETHZ

Meeting modern challenges in engineering require an understanding of the flow phenomena in complex, multicomponent fluids in a wide range of scales, starting from turbulent flows to flows at a micron scale where the traditional continuum mechanics approach becomes invalid. These challenges are mirrored in the development of modern computational approaches which have to tackle multi-scale physics in simulation.

The goal is to significantly advance the development of a particularly promising approach – the Lattice Boltzmann Method – and to bring it to a ready-to-use state for engineering applications.

Main Investigator
Ilya Karlin, ETHZ

Project Partners
ETHZ (LAV, LTNT)
EPFL
PSI
Empa

This methodology occupies an intermediate place between the purely continuum mechanics on the one hand and the molecular dynamics on the other.

In the course of this project, the framework of the Lattice Boltzmann approach to modelling of complex flows has been significantly extended in three directions: simulation of turbulent flows, simulation of thermal flows with high temperature and density variations, and multi-component mixtures, including surface-based chemical reactions. These newly developed models and state-of-the-art computational realizations enable simulation of systems with multiple scales.

PSI

A multispecies, non-isothermal Lattice Boltzmann (LB) code was developed and tested on catalytic channels. The new model can also be used in the micro-flow simulation of mixtures in the slip-flow regime. At the same time an intensive study has been initiated to develop a tool allowing the direct simulation of the flow inside a porous media using the geometrical reconstruction obtained experimentally by Empa.

A full LB code for catalytic reactions in porous media is expected to be ready within 2008. The end of 2008 is the expected milestone for the application of the code to more realistic microreactors (full chemistry).

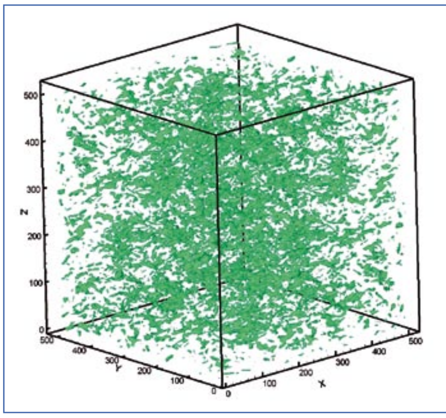
LTNT-ETHZ

The first goal of LTNT within this project is the study of the fuel processing in micro reactors, particularly the production of syngas from hydrocarbons. The second goal of the project is the numerical simulation of the chemically reactive flow and the electrochemistry in the anode side of a SOFC.

Our results showed that the herein presented reactor configurations may well be suited to provide small and portable butane processing units for applications together with micro fuel cells.

One of the conclusions of the study so far, is that the better understanding of butane-to-syngas conversion requires more detailed numerical simulations of our experiments based on an extension of the existing numerical models. The simulations should include mass flow through the porous medium and complex reaction mechanisms since the catalytic reactions of butane on rhodium surface are evidently more comprehensive than those of methane.

EPFL



Entropic Lattice Boltzmann simulation of the three-dimensional Kida-vortex flow at Re=20000. Iso-vorticity surfaces at the peak of enstrophy are presented on a 512x512x512 grid.

Despite the advantages of fuel cells there are several factors impeding their market penetration.

Commercial natural gas and other hydrocarbon fuels contain traces of components present as impurities or even additives (as odorants due to safety regulations) that act as catalyst poisons and can dramatically affect the performance of the fuel cell. Sulfur is the most prominent contaminant in this context. Sulfur not only suppresses the electrocatalytic properties of the Ni in the cermet, but also affects its thermal and redox stability.

This work focuses on fuel related issues applicable to fuel cell electrodes and, in particular direct reactions of fuels on SOFC anodes, electrode deactivation, electrode and catalyst poisoning and recovery of the lost catalytic activity. The first priority is to prevent degradation of SOFC anodes by contaminants such as sulphur present in the fuel.

The work performed under this CCEM project establishes the achievement of a strikingly higher level of protection of the cermet against sulfur deactivation and corrosion than that achieved previously with the conventional hydrodesulfurisation (HDS) catalysts. It has even been shown that with modifying Ni-YSZ anode by the addition of a new catalyst, it is possible to operate it under fuel containing considerable percentages of sulfur containing compounds and thereby eliminate the desulfuriser from the SOFC system. Experimentally the sulfur has been added as either thiophene or H_2S into the fuel stream to validate this claim. The new invention has another considerable advantage in the sense that the said catalyst could be added with minimum modifications to the cell fabricating protocols. This avoids elaborate procedures and cost multiplying additional steps.

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Empa

The Fast Ion Conductors group at Empa's Laboratory for High Performance Ceramics is involved in a number of research projects and collaborations, that address various issues on cathodes, electrolytes and anodes of solid oxide fuel cells. Our role in the CEMTEC CCEM project is to provide the project partner LAV ETHZ with experimental structure parameters of SOFC cell assemblies that enter their LB models.

Two sets of solid oxide fuel cell (SOFC) electrode assemblies from different manufacturers were run under different operation conditions with different sulfur exposure, and then subject to sulfur (1s) x-ray absorption spectroscopy (XAS). Within the detection limits of the spectrometer, pristine anodes show no sulfur at all. The electrodes operated with sulfur containing natural gas and H_2S doped natural gas show similar spectra, which were rich in sulfur structures, the most prominent of which being sulfate and thiophene. Two other electrodes run with sulfur containing natural gas, one plus a sulfur filter and the other without filter showed an XAS spectrum with a very broad peak, covering the entire sulfur absorption range, and thus not allowing for identification of one or more specific sulfur signatures.

These appear to be the first ever reported sulfur XAS data on SOFC anodes, and the XAS technique keeps promise to resolve some hitherto unresolved issues on sulfur poisoning of SOFC anodes, particularly the molecular speciation of the sulfur.

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