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Pore-resolved Simulation of Energy Conversion in Novel Porous Media Designs

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About Me

Academic background

- Bachelor's and master's in **chemical engineering and process engineering** at the Karlsruhe Institute of Technology
- Researcher at the Steinbuch Centre for Computing and Engler-Bunte-Institute, studying **combustion processes**
- In 2019**, 3 months research** stay at Jiangsu University and Peking University, China, working on joint energy systems projects

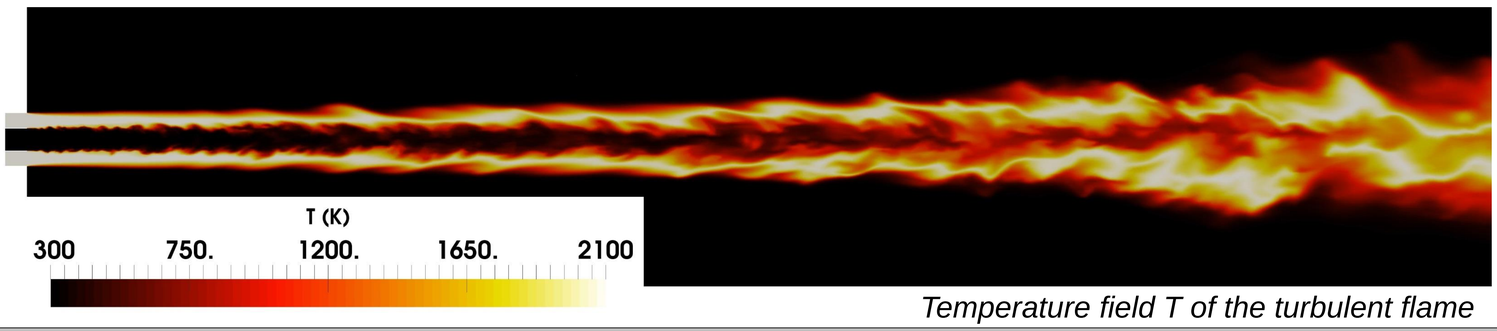
Personal interests

- High Performance Computing: developing highly efficient code for simulations on the **world's largest supercomputers**
- **Detailed modeling** of physics: molecular diffusion and chemical reaction kinetics

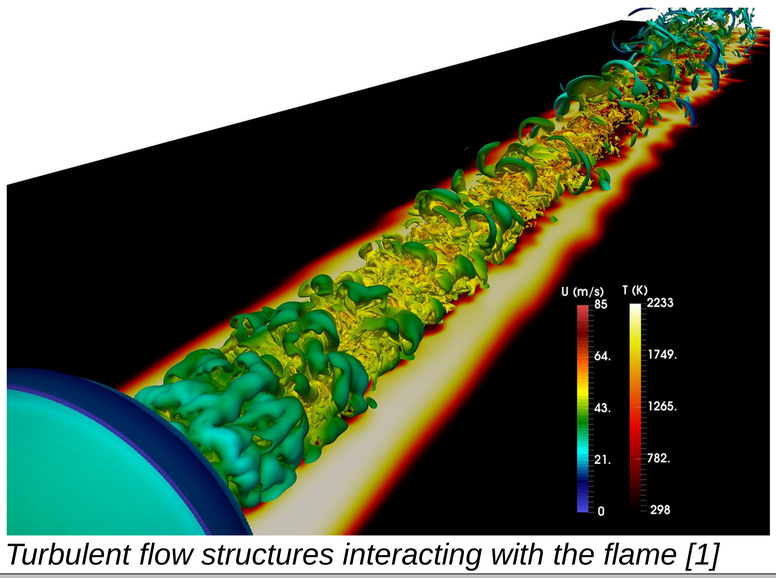
Past Research Highlight

Large-scale simulation of turbulent flames [1]

- Detailed simulation on Germany's largest supercomputer of an experimentally investigated flame
- 19 chemical species, over 200 elementary chemical reactions, 150 million cells, 30,000 CPU cores
- 10 TB database for the development of new combustion models



Temperature field T of the turbulent flame

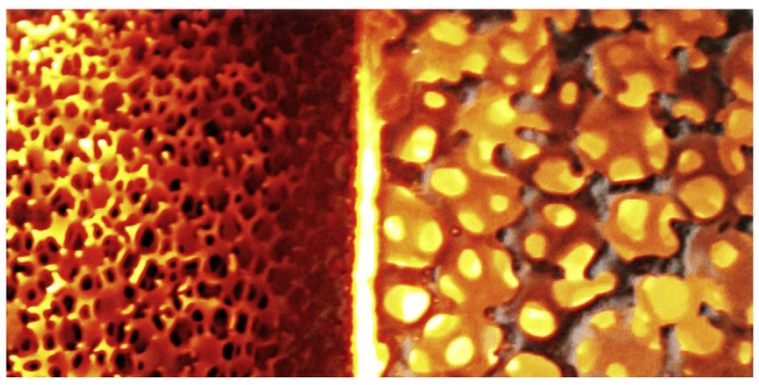


Turbulent flow structures interacting with the flame [1]

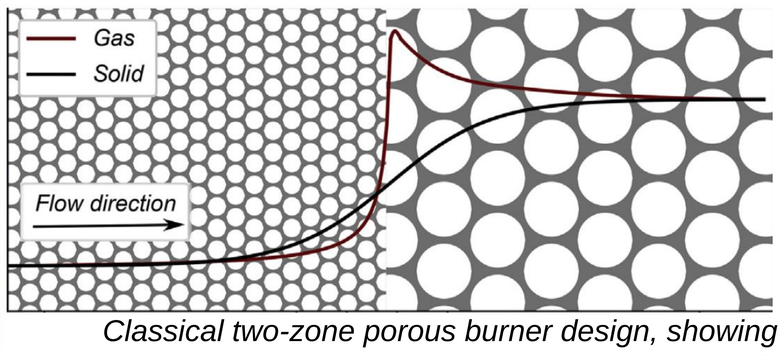
DAAD PRIME Research Proposal

Motivation

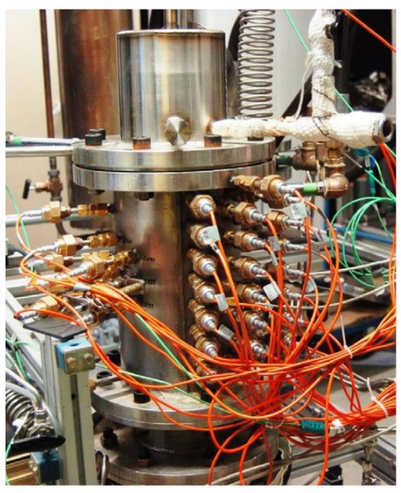
- To reduce **pollutant emissions** in the future, more efficient energy devices must be developed
- Energy conversion in **porous media** is a promising concept for **sustainable** energy supply
- Large heat conductivity of the solid matrix and the high contact area between gas and solid in micro-pores increase the **range of operability** and leads to **drastically reduced emissions**
- Porous media systems also show good potential for reformers for future **hydrogen production**

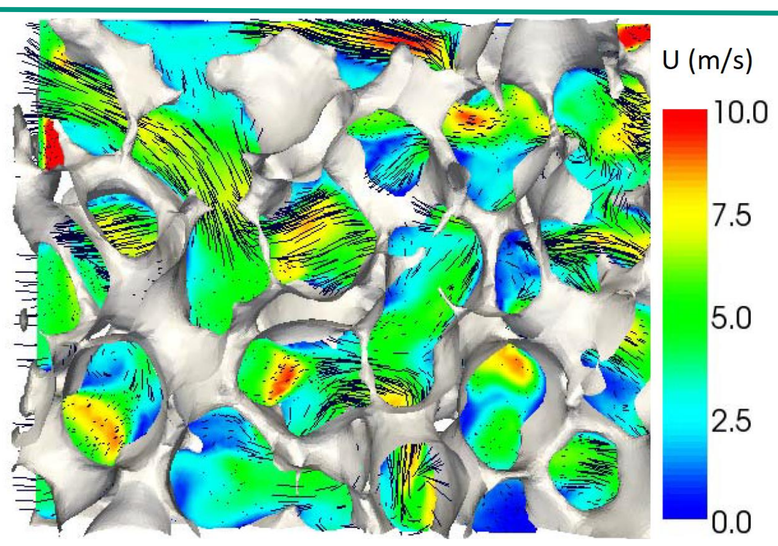


Flame burning within a solid matrix [2]



Classical two-zone porous burner design, showing temperature profiles of solid and gas [2]





Experimental setup for a porous media burner at KIT (left) and simulation of flow through a porous matrix [3]

Research goals

- Perform the **most detailed simulations** of energy conversion in porous media on supercomputers
- Implement **state-of-the-art numerical models**
- Simulations based on real geometries created with **cutting-edge 3D printing techniques** at Stanford
- Validation with 3D tomography results
- Advance the **fundamental understanding** of reacting flows in porous media
- **Optimize the pore structure** to enable the most efficient use for reformers and burners
- Derive simplified one-dimensional models to aid the **design of new porous media systems**

[1] T. Zirwes et al., *Flow, Turbulence and Combustion*, volume 104, 997–1027 (2020)
[2] D. Mohaddes, C. T. Chang, and M. Ihme, *Energy*, volume 207 (2020)
[3] C. Bedoya et al., *Energy Technology*, volume 5, 1124-1133 (2017)

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