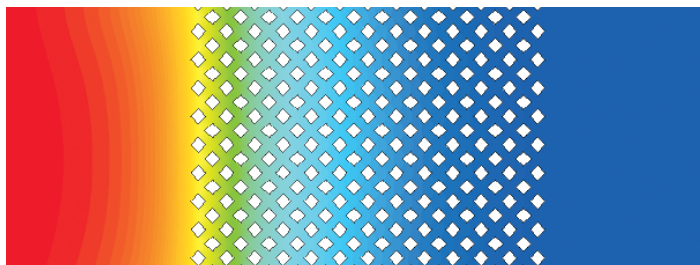
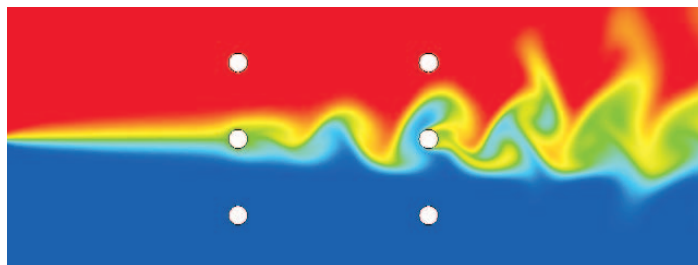


The Power of Microreactors

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Ammonia mass fraction contours along a post microreactor indicating axial dispersion-like behavior at low flow rates



Enhanced mixing in a post microreactor at moderate Reynolds number due to vortex shedding ($Re = 100$, post diameter, $d=200 \mu\text{m}$, and inter-row spacing = $10d$)

THE USE OF PORTABLE ELECTRONIC DEVICES, including cellular phones, laptop computers, global positioning devices, and electrically powered vehicles continues to grow rapidly. This growth necessitates the development of lightweight, efficient, and portable power generation devices. Currently, this miniaturization is severely limited by the low efficiency of traditional batteries. Hydrogen-based fuel cells offer an appealing, relatively high efficiency alternative, using the conversion of high energy density hydrocarbons to electricity. Challenges with hydrogen storage and safety, however, mean that on-board hydrogen production for fuel cells is a must. Alternative paths to electricity, whereby a microcombustor is integrated with a thermo-electric or photovoltaic device, are also being explored.

Miniaturization of large scale reactors requires a re-thinking of how to scale-down devices. For example, catalyst in the form of particulates, which has traditionally been used in fixed bed reactors, would create an unacceptably large pressure drop and fluid bypass in sub-millimeter, portable devices. In addition, more active catalysts and better heat transfer are needed to ensure rapid response in frequent start-up and shut-down operations. Another factor that limits scale-down is mixing, which is limited to inherently slow molecular diffusion. These issues highlight the fact that relatively open, monolithic microstructures with enough catalyst embedded in them are needed for miniature portable power generators.

At the Center for Catalytic Science and Technology (CCST) at the University of Delaware, FLUENT is

being used to explore different designs of microstructured reactors for energy generation. In order to develop better catalysts, detailed surface reaction mechanisms are needed. Parameters are first estimated using semi-empirical techniques and are then improved in a hierarchical multiscale manner using quantum mechanical density function theory (DFT) [1]. Since DFT is computationally intensive, it is carried out for the important reactions and for the most abundant surface intermediates only. These important reactions and key species are identified using sensitivity and reaction path analyses in simple plug flow reactors that are much cheaper to run. Molecular dynamics with potentials obtained by DFT [2] and kinetic Monte Carlo simulations with DFT energetics may also be run during hierarchical multiscale model development [3]. Eventually, detailed surface reaction mechanisms, reduced rate expressions, or even neural network parameterizations of these are interfaced with FLUENT to enable the simulation of microreactors [1].

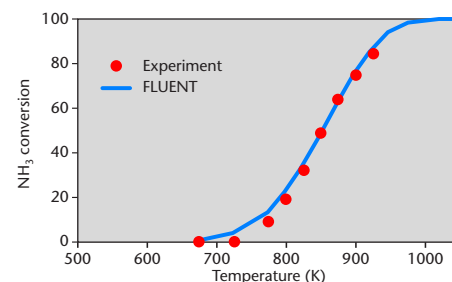
A number of post microreactors for hydrogen production via ammonia decomposition are currently being studied. An example of an actual microreactor is an array of 11 (y-direction) x 25 (x-direction) square posts. The catalytic posts are arranged in a 45° rotated configuration, and surface reactions occur on the post surfaces. (Mass transfer inside the posts is neglected.) Pure ammonia flows in through the inlet at uniform velocity, and following surface reactions on the posts, is converted to hydrogen.

FLUENT's laminar flow model is being used for the simulation with a 2D mesh of over 150,000 elements, with finer resolution near the post surfaces.

The chemistry model is coupled with the segregated solver using a user-defined function (UDF) to simulate ammonia decomposition. The model predictions for conversion are in good agreement with published experimental data [4]. In particular, the analysis reveals enhanced external mass transfer due to the posts. ■

References

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Model predictions for ammonia conversion as a function of temperature are in good agreement with experimental data in the post microreactor