SAND2016-0341C

Chemically Reacting Flow Through Additively Manufactured Structures

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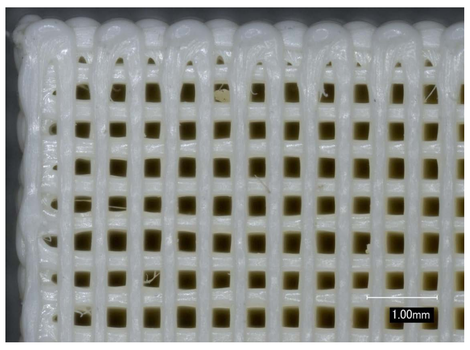
Introduction

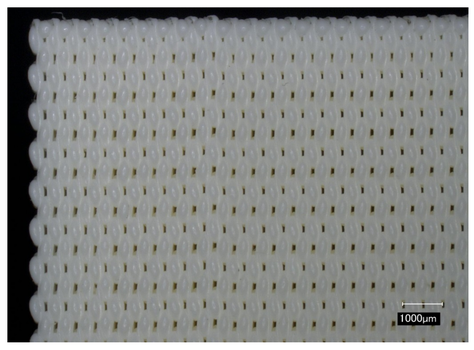
Additive manufacturing is heralded by mechanical engineers as a new path to load-bearing structures that use material very efficiently. The emerging field also has promise in chemical engineering, where there is a ubiquitous reliance on randomly packed powders in chemical reactors; separator membranes for batteries and fuel cells; separation columns; and other devices that manipulate fluid flow and ion transport. Replacing randomly arranged materials by deterministically fabricated devices with optimized geometries achieves major performance and efficiency improvements. Notable examples can be found in gas chromatography, microfluidic medical devices, and recently emerging "3D battery" structures. We are working to model an additively manufactured exchange chromatography column to gain a quantitative understanding of the potential benefits of the geometries made possible by 3D printing.

Additive Manufacturing Technologies

The most widespread 3D printing technologies involve rastering an extruder or heat source to draw lines in a plane, followed by drawing of additional planes. Pore space can be created by adding a soluble support material, or by bridging short gaps. A “logpile” structure can be printed easily at near the resolution limit of the printer, often without support material, which can be difficult to remove from long, narrow pores.

The structure shown below was printed using a Stratasys Fortus 400 printer at SNL/CA using ABS plastic. The left image is the top view. Both of the side views look like the right image. Sides are occluded by the loop of material caused by changing raster direction.





Channel pitch = 1 mm

We are interested in flow through different orientations of this structure, notably the “111” orientation, where all flow paths face a similar pressure drop.

Exchange Chromatography Column

Exchange chromatography is of scientific interest because the second-order chemical reaction between phases results in a theoretically infinitely sharp boundary that does not broaden as it progresses, although broadening mechanisms do occur in practice, and are easily studied. In our case, we examine the exchange of hydrogen and deuterium with a hypothetical 3D-printed metal hydride column.

Laminar gas flow and convection-diffusion in gas phase:

$$\frac{\partial H}{\partial t}+\nabla\cdot\left(H\,\boldsymbol{u}-D_g\nabla H\right)=0$$

The velocity field ***u*** is obtained by solving the Navier-Stokes equation

Diffusion in the solid phase:

$$\frac{\partial H_s}{\partial t}-\nabla\cdot\left(D_s\nabla H_s\right)=0$$

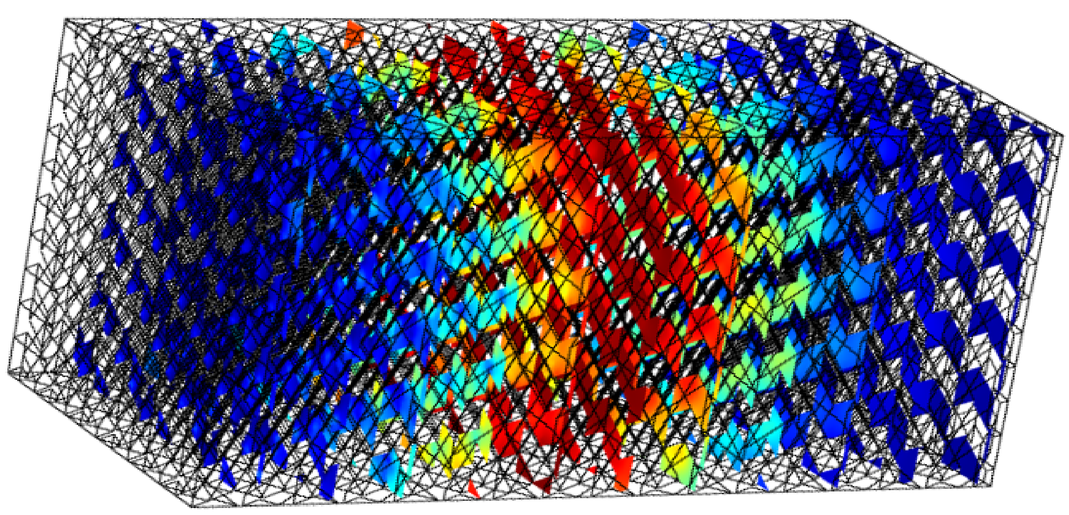
Flux at the solid-gas interface (second-order chemical reaction):

$$\Phi=\alpha\,k\left(H/C_g\right)\left(1-H_s/C_s\right)-k\left(H_s/C_s\right)\left(1-H/C_g\right)$$

C_g and C_s are the gas and solid capacities

Preliminary Results

Finite-element computations allow the simulation of reactive flow through a 111 logpile column as a function of its geometric parameters such as channel pitch, flow orientation, pressure drop, etc.



Reaction front, as indicated by diatomic HD concentration (red=high, blue=low), in a “logpile” structure with flow along the “111” orientation (1 cm long, channel pitch = 1 mm)

Reaction front in a 1D column (1 cm long, radius = 50 µm)

Summary and Future Directions

Our preliminary results suggest that a front can be obtained in a hypothetical 3D structure and that it is comparable to the front predicted in a 1D structure. Future work will involve comparing columns of 3D flow structures with an array of 1D columns with a given diameter tolerance. We expect that the array will result in broad fronts in the total flow due to varying flow rates between the tubes, whereas the 3D structure will allow mixing between inhomogeneous regions, maintaining a sharp front.

U.S. DEPARTMENT OF ENERGY

National Nuclear Security Administration

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SAND No. 2011-XXXXP