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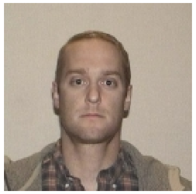
SAND2021-5455C

Fluid flow control devices with 3D-graded permeability



PRESENTED BY

David B. Robinson

Maher Salloum, Denis Ridzal, Drew P. Kouri

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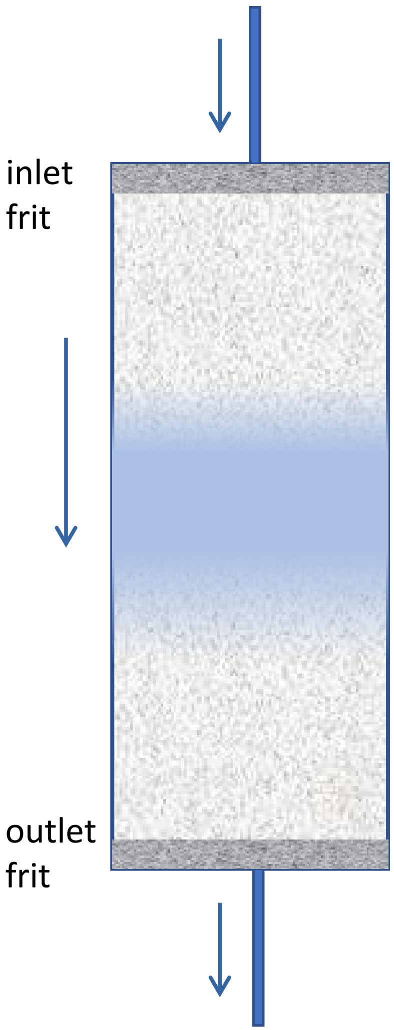
Background and Motivation



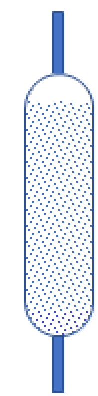
Chemical engineering systems such as chromatography and catalyst columns often rely on porous media.

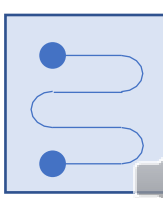
Microscopic pore geometry defines macroscopic permeability, defining flow rate versus pressure.

Fluid phase can travel over varying cross sections or around corners, where flow can be nonuniform.

Examples:

- Stainless steel columns with frits
- Glass columns with hemispherical ends
- Column on a chip





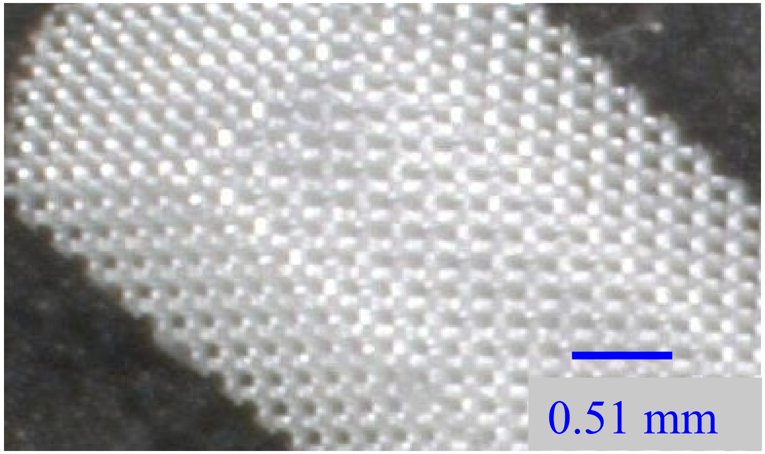
Challenge: Adjust permeability to maintain spatially uniform fluid velocity despite nonuniform geometries.

3D Printing of Porous Material

Additive manufacturing (AM) techniques raise the possibilities that porous media can be fabricated in which the permeability can be arbitrarily specified in three dimensions

By varying laser power and speed, and tuning particle size distribution, Mott Corporation has claimed the ability to spatially vary permeability using metal laser sintering AM methods.[1]

We have previously studied flow through additively manufactured polymer lattices with precisely defined pores.[2,3]



1. V.P. Palumbo et al. "Porous Devices Made by Laser Additive Manufacturing." US Patent Application 2017/0239726 A1, Mott Corporation, 2017.
2. M. Salloum and D.B. Robinson "A Numerical model of exchange chromatography through 3-D lattice structures", *AIChe J.* vol 64(5), pp. 1874-1884, 2018
3. D.B. Robinson. 3D-Printed Apparatus for Efficient Fluid-Solid Contact. US Patent 10493693 B1 (2019).

Permeability and Porosity, Pressure and Flow

We focus on Darcy's Law:

- Assumes slow flow
- Applicable scale: pore < L <= column

$$v = \frac{\kappa}{\mu L}\Delta p$$

v = fluid velocity $\left(\frac{\text{m}}{\text{s}}\right)$
κ = permeability $\left(\text{m}^2\right)$
μ = viscosity (Pa s)
L = length (m)
Δp = pressure drop (Pa)

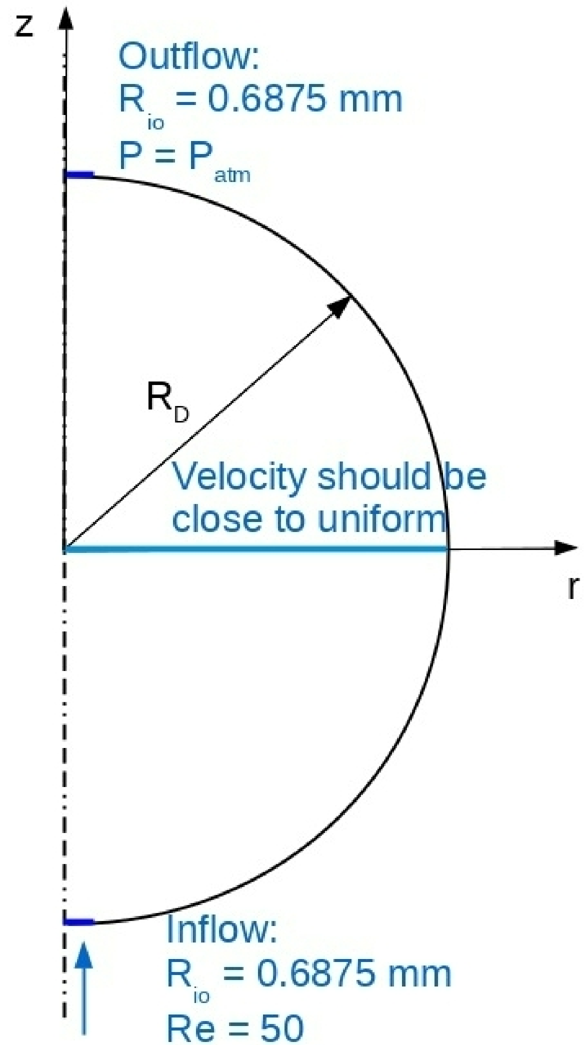
Permeability is related to porosity ε (pore volume fraction)

- Depends on pore geometry and how it is changed
    - Compaction, sintering, 3D printing, etc.
- Square array of circular pipes, fixed spacing W:
  $\kappa = \frac{W^2\varepsilon}{8\pi}$ for $0 < \varepsilon < \pi/4$
- Packed spheres, diameter D: Kozeny-Carman equation
  $\kappa = \frac{D^2\varepsilon^3}{150(1-\varepsilon)^2}$
- See Erdim et al., Powder Tech. 283 488 (2015)

10x κ variation seems plausible

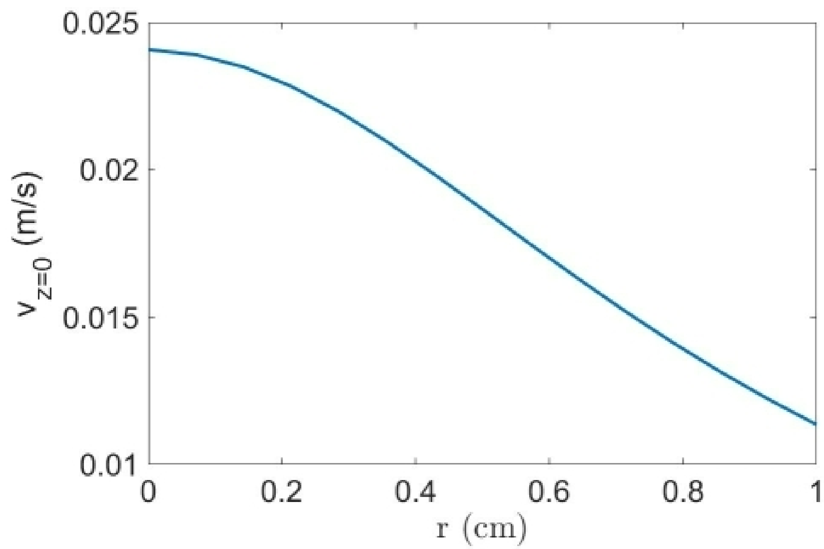
Spherical Column Geometry

A spherical column is a simple model of a glass column with hemispherical ends.



We start by studying a sphere of axi-symmetric model geometry.

For a constant permeability of 10^{-12} m/s, the resulting midplane velocity profile is:



We seek a graded permeability that meets criteria such as a uniform flow velocity mid-way between the inlet and outlet, or uniform transit times along streamlines.

Spherical Column with Graded Permeability

Iterative Optimization

In our optimization, we do not impose any functional form of the permeability field.

We obtain the optimal solution iteratively by adjusting the permeability field model input according to the midplane velocity and transit time results at each iteration.

We start with a constant permeability $K=K_0$ and repeat the following until convergence:

$$K(r,z)_i = K(r,z)_{i-1} \cdot \frac{max[v(r)_{i-1}]}{v(r)_{i-1}} \cdot \frac{\tau(r,z)_{i-1}}{max[\tau(r,z)_{i-1}]}$$

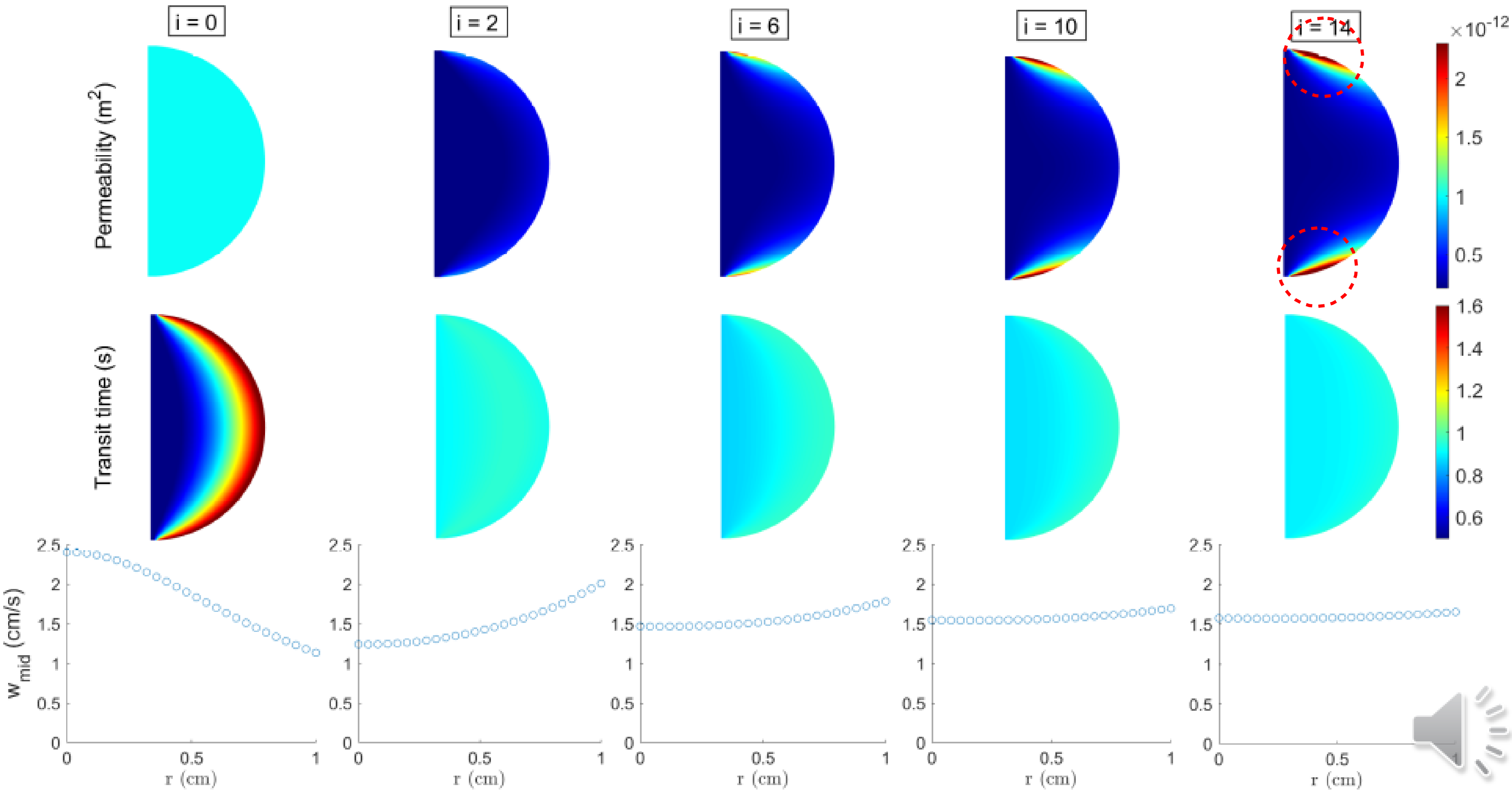
This algorithm adjusts the local value of the permeability according to the midplane velocity at that radius and transit time on that streamline.

Spherical Column with Graded Permeability

Optimization Results

An optimal solution is obtained within 14 iterations with uniform velocity and transit time.

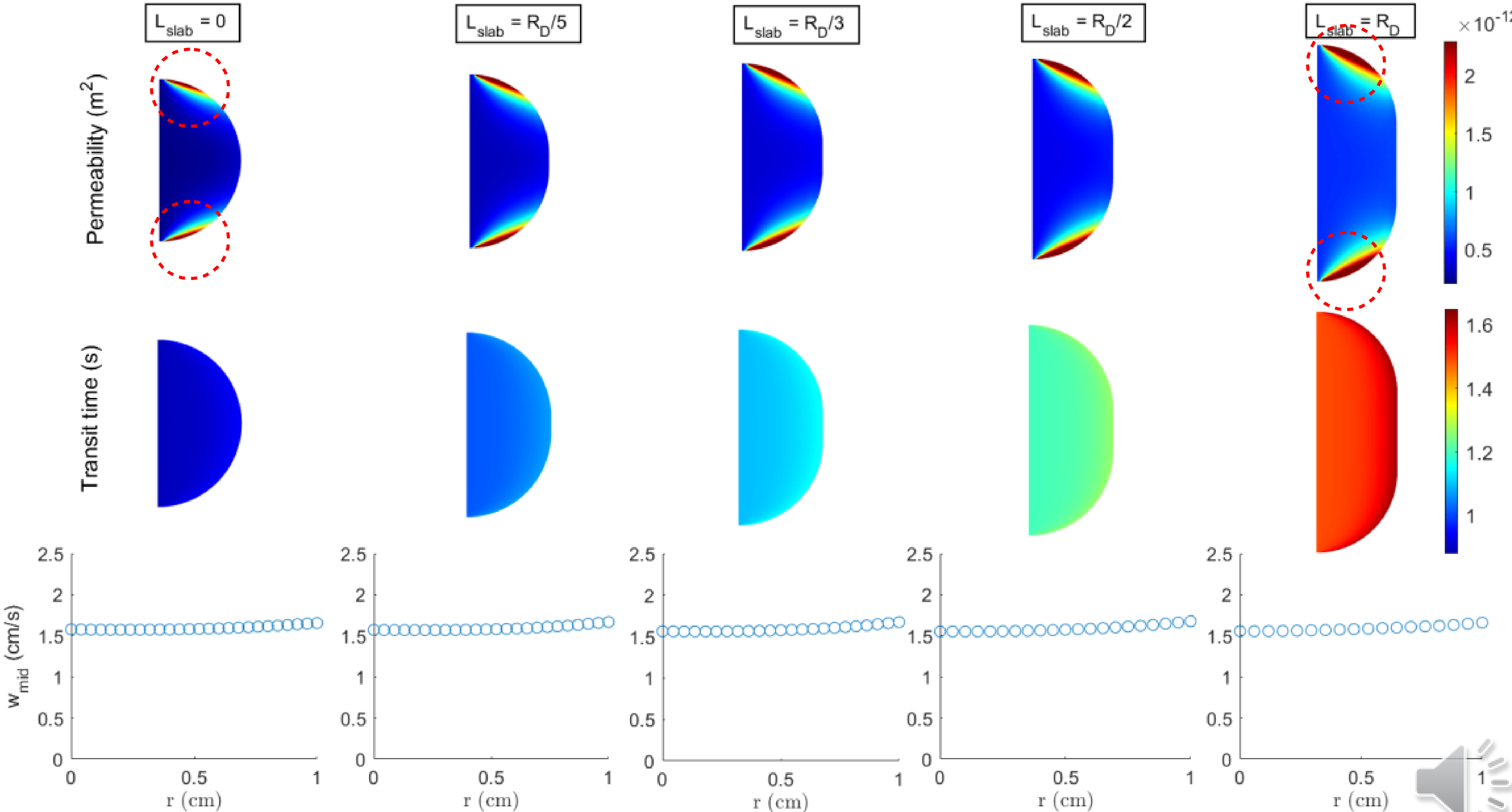
By grading the permeability only near the sphere inlet and outlet over a 10x range, we obtain uniformity in midplane velocity and transit time within about 10%.



Spherical Column with Graded Permeability

Effect of an Inserted Slab

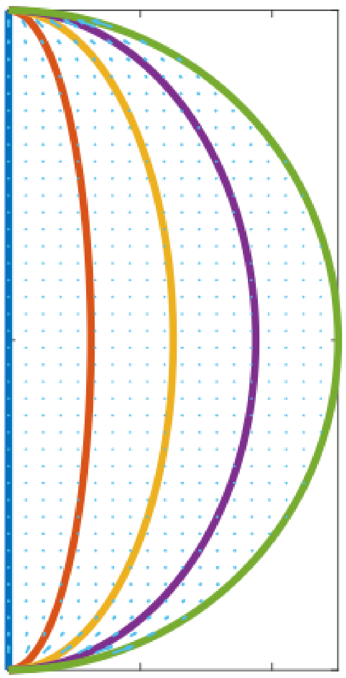
Similar permeability field trend is obtained for a slab inside the sphere which simulates a more cylindrical geometry (e.g., glass chromatography column)

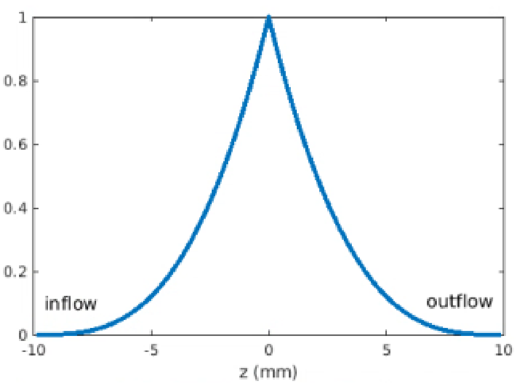


Velocity Field Optimization

Trust-region Newton method is a more general optimization scheme (see references).

We use it to pursue specified analytical velocity fields.





We prescribe the ***desired*** velocity field as

$$v_r(r,z) = \frac{-\beta r z}{(R^2 - z^2)^2} \quad \text{and} \quad v_z(r,z) = \frac{\beta}{R^2 - z^2}$$

where β is a constant that we also optimize for.

Features include:

- v_z depends only on z, keeping transit time uniform.
- Uniform midplane velocity.
- Divergence-free for |z| < R.
- Streamlines keep same ***relative*** distance from central axis.
- Ignores complexity near inlet and outlet.

Weighting: We minimize the misfit between a ***simulated*** velocity, given by Darcy's law, and the ***desired*** velocity. We use a **cubic weighting** to deemphasize large inlet and outlet velocities.

C. J. Lin and J. J. More. "Newton's Method for Large Bound-Constrained Optimization Problems." SIAM J Optim. 9 (4) 1100-1127, 1999.
T. Borrvall, J. Petersson. "Topology Optimization of Fluids in Stokes Flow." Int. J. Numer. Meth. Fluids 41, 77–107, 2003.
M. A. Heroux, R. A. Bartlett et al. "An overview of the Trilinos project." ACM Trans. Math. Softw. 31(3), 397-423, 2005

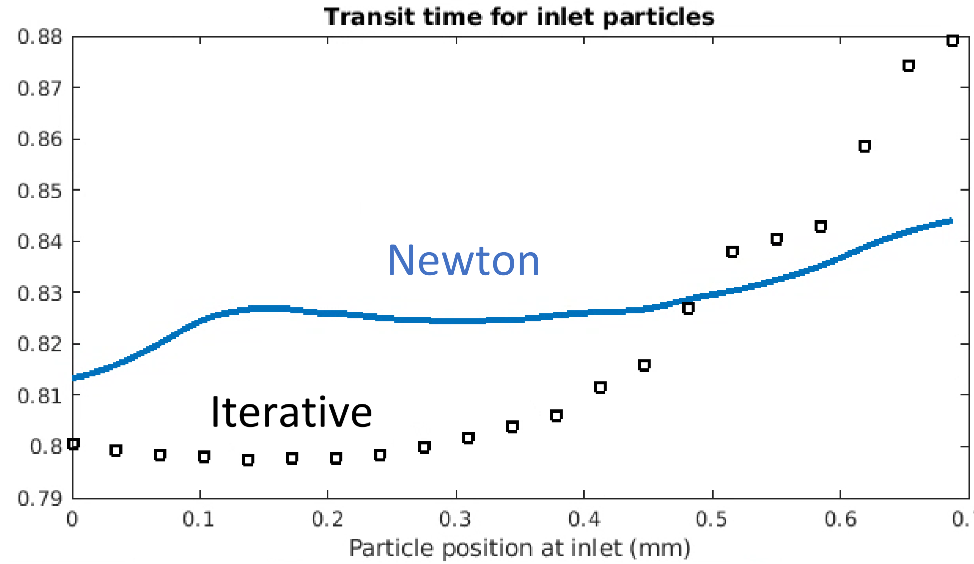
Velocity Field Optimization Results

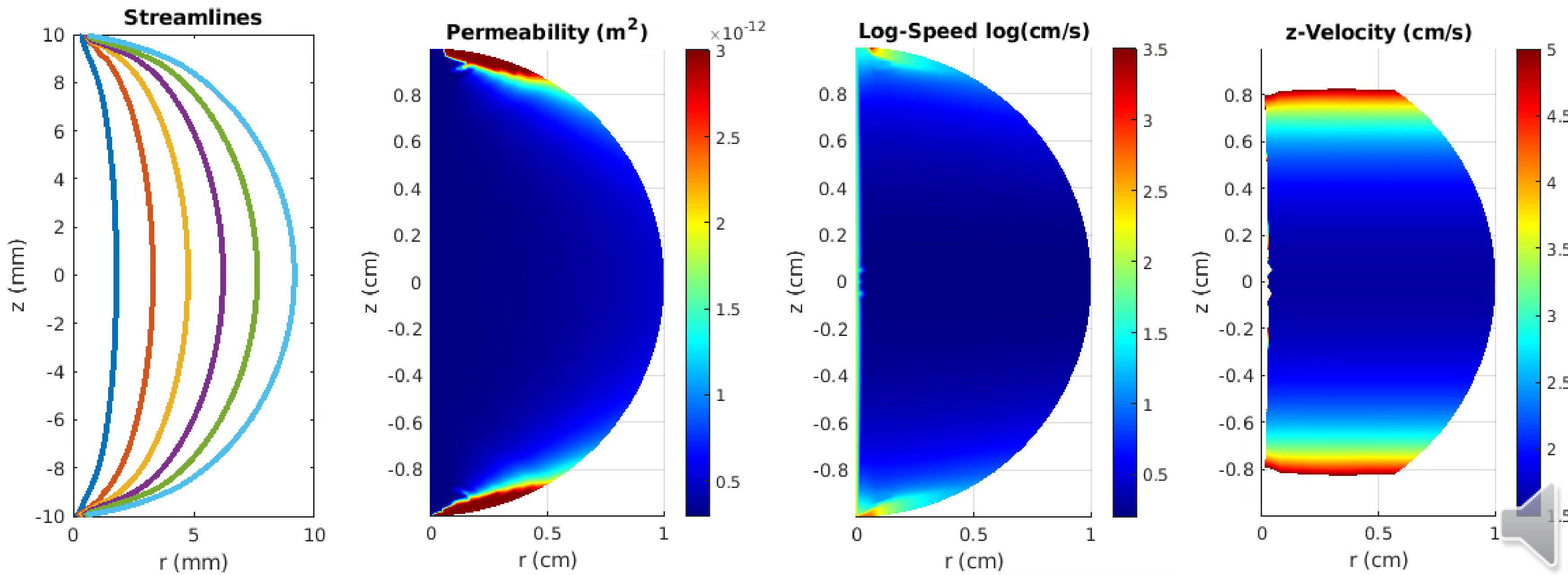
Optimization of velocity field by trust-region Newton method improves transit time uniformity versus our iterative method.

Streamlines closely match target shape.

Permeability is graded mainly near inlet and outlet, as for iterative method.

Midplane velocity is uniform to about 0.1%.





Conclusions

Additive manufacturing techniques may enable novel architectures for porous media.

Optimized graded permeability can achieve desired fluid velocity fields and transit times in flow columns.

Our optimization methods yield solutions that improve flow uniformity in spherical columns.

Spherical columns with uniform transit time could be easily manufactured by simply grading permeability in regions near the inlet and outlet.

Adding a slab in the middle of a spherical column approximately preserves the optimal graded permeability field.

Acknowledgements and Contact Info

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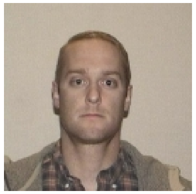
Dave Robinson,
drobins@sandia.gov
www.sandia.gov/drobins

Maher Salloum

Denis Ridzal



Drew Kouri

Live presentation:
2 Jun 2021
16:00 CET