Sandia National Laboratories

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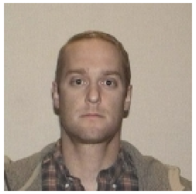
Fluid flow control devices with 3D-graded permeability



PRESENTED BY

David B. Robinson

Coauthors: Maher Salloum, Denis Ridzal, Drew P. Kouri, David J. Saiz and Bradley H. Jared

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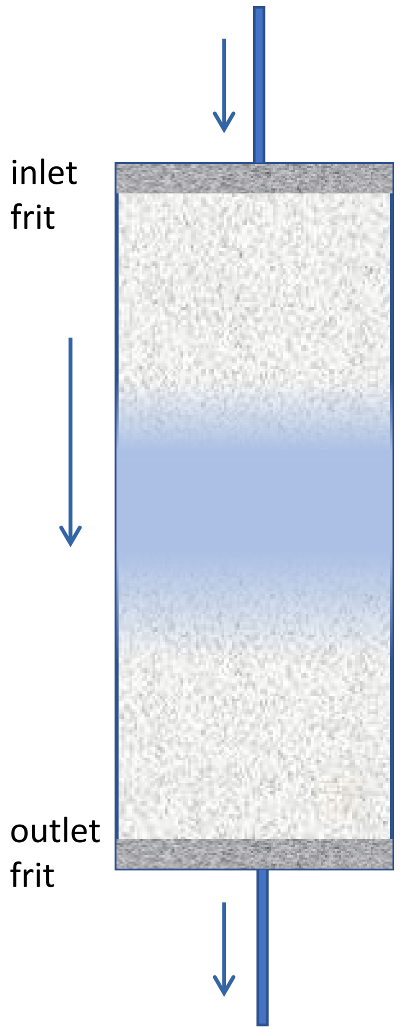
Background and Motivation



Chemical engineering systems such as filters, catalytic reactors and chromatography often contain components made of porous media

Often the fluid travels over varying cross sections, especially near the inlet and outlet, where flow can be nonuniform.

Examples of applications

Mixture analysis
Bulk separation
Ion exchange

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

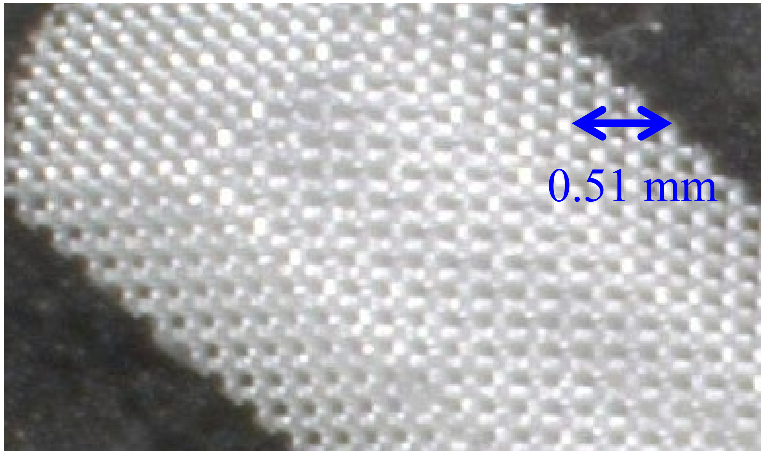
3D Printing of Porous Material

Hypothesis: Varying the spatial permeability can achieve uniform fluid velocity through porous media despite nonuniform geometry.

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 laser sintering AM methods.[1]

At AIChE 2016, we described models of flow through additively manufactured lattices with precisely defined pores.[2]



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

Case Study

Spherical Columns (or Hemispherical Ends)

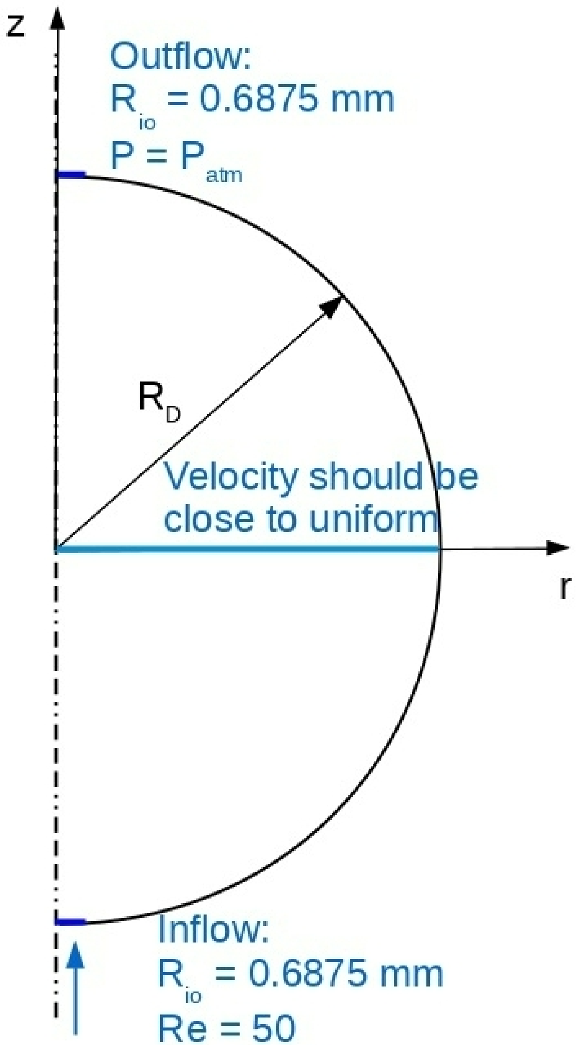
Inert porous frits abruptly change flow diameter at inlet and outlet in cylindrical columns.

- Sharp corners cause large stresses around the device inlet

Curved regions such as spherical shapes could decrease stress concentrations in high-pressure chromatography, and increase the amount of active porous material.

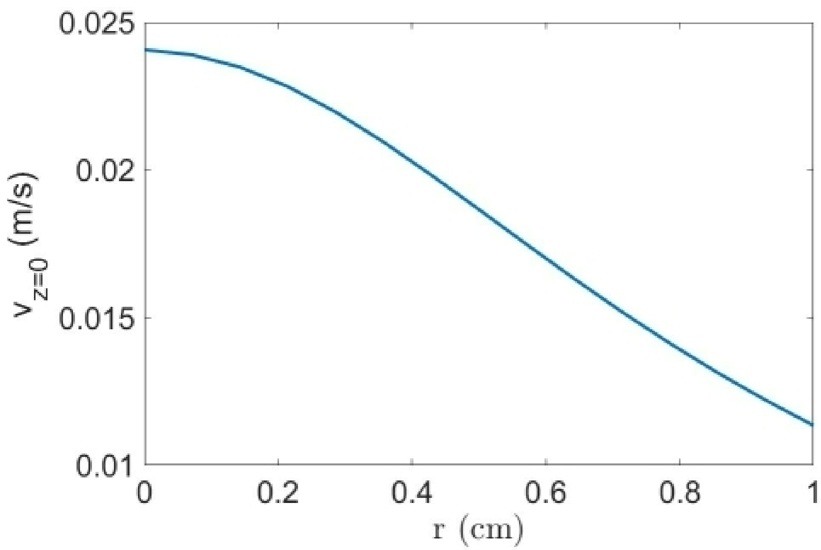
We would like to study the feasibility of graded permeability of spherical porous columns through an optimization study using a simple Darcy flow model and more complex models.

Spherical Column Geometry



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

For a constant permeability $K_0 = 10^{-12}$ m/s, the resulting midplane velocity profile is:

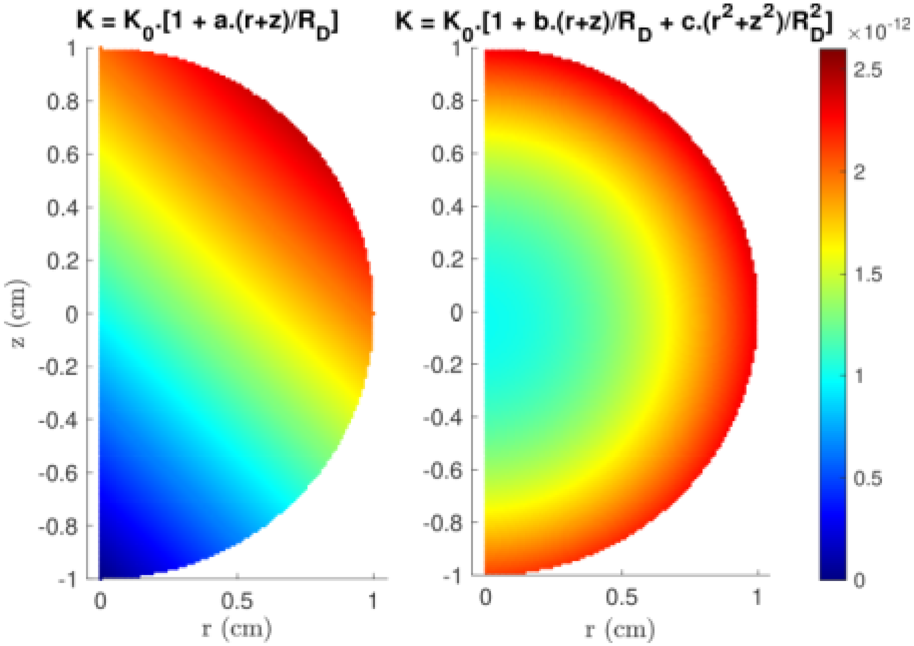


We seek a graded permeability that establishes a uniform flow velocity mid-way between the inlet and outlet.

Spherical Column with Graded Permeability

Parametric Optimization

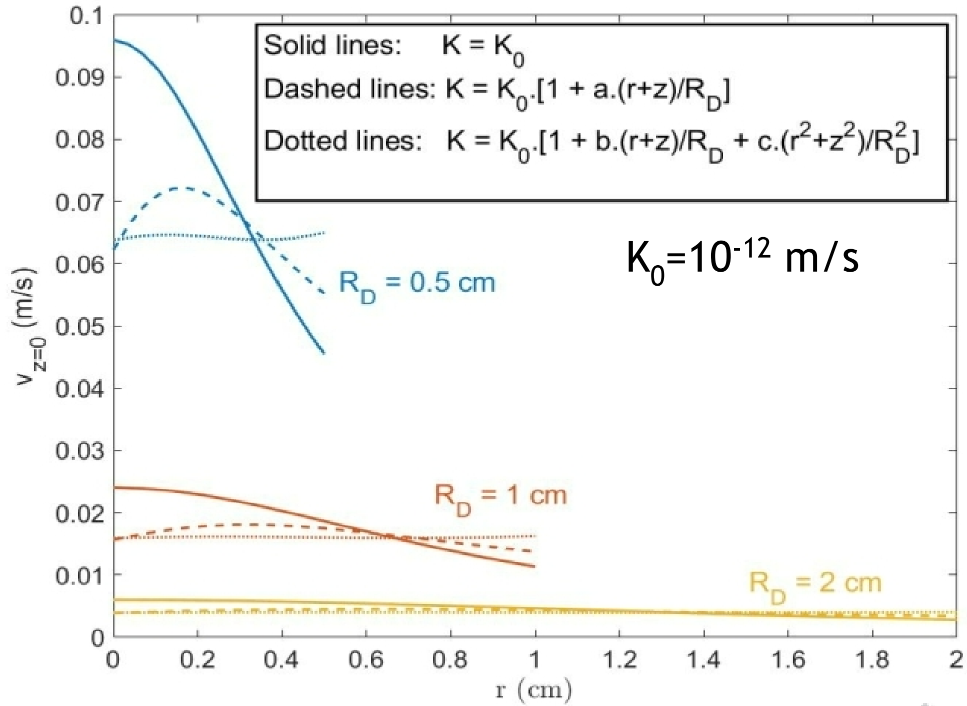
We assume linear and quadratic permeability profiles ($K_0=10^{-12}$ m/s)



R_D = 1cm

The contribution of the linear term vanishes when a quadratic term exists

A quadratic term is necessary to obtain a nearly uniform velocity profile

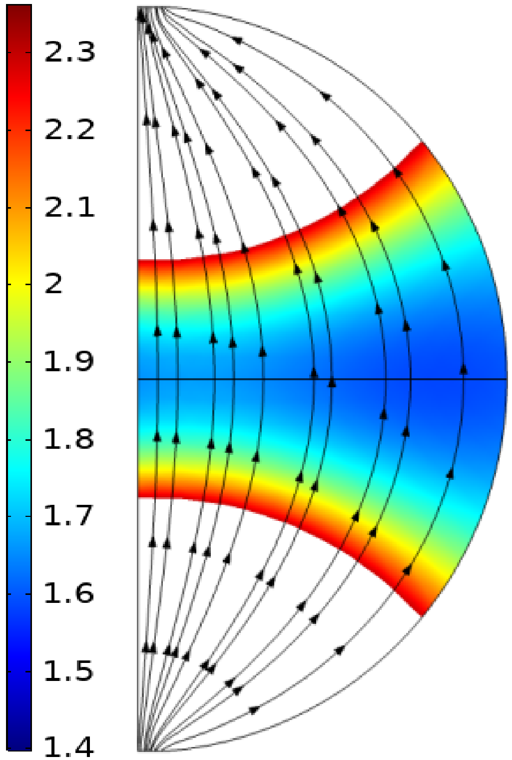


Spherical Column with Graded Permeability

Parametric Optimization – Transit Time

Although a uniform velocity profile is obtained in the sphere mid-plane, the transit time along the flow streamlines is still not uniform.

Streamlines and velocity field (cm/s)

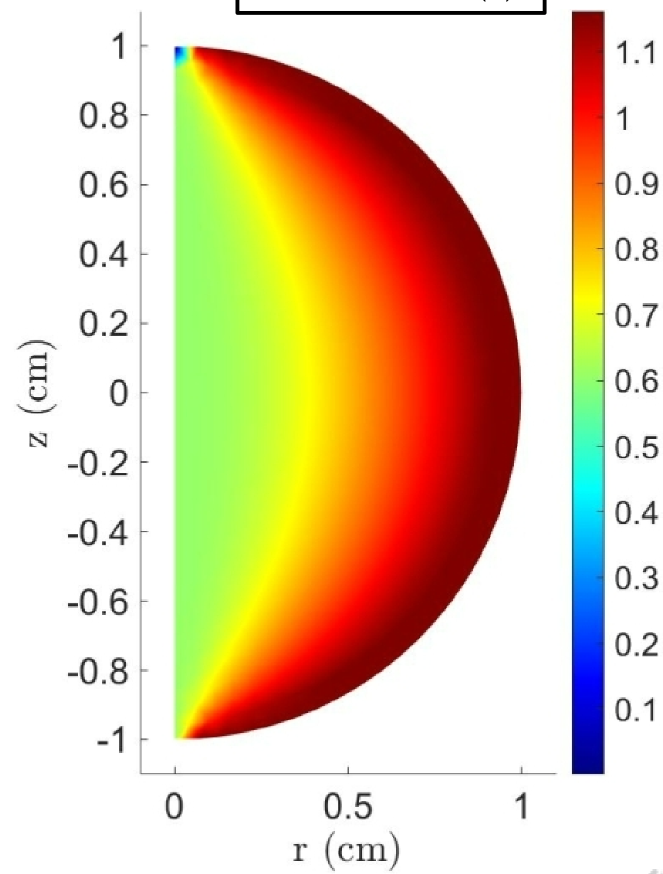


We define the transit time τ as the time taken by a fluid element to travel along a streamline.

We also seek a uniform transit time among all of the streamlines.

This could allow a chromatography peak to remain sharp at the outlet.

Transit time (s)



Spherical Column with Graded Permeability

Iterative Non-Parametric Optimization

In non-parametric 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 velocity profile and transit time output.

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

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

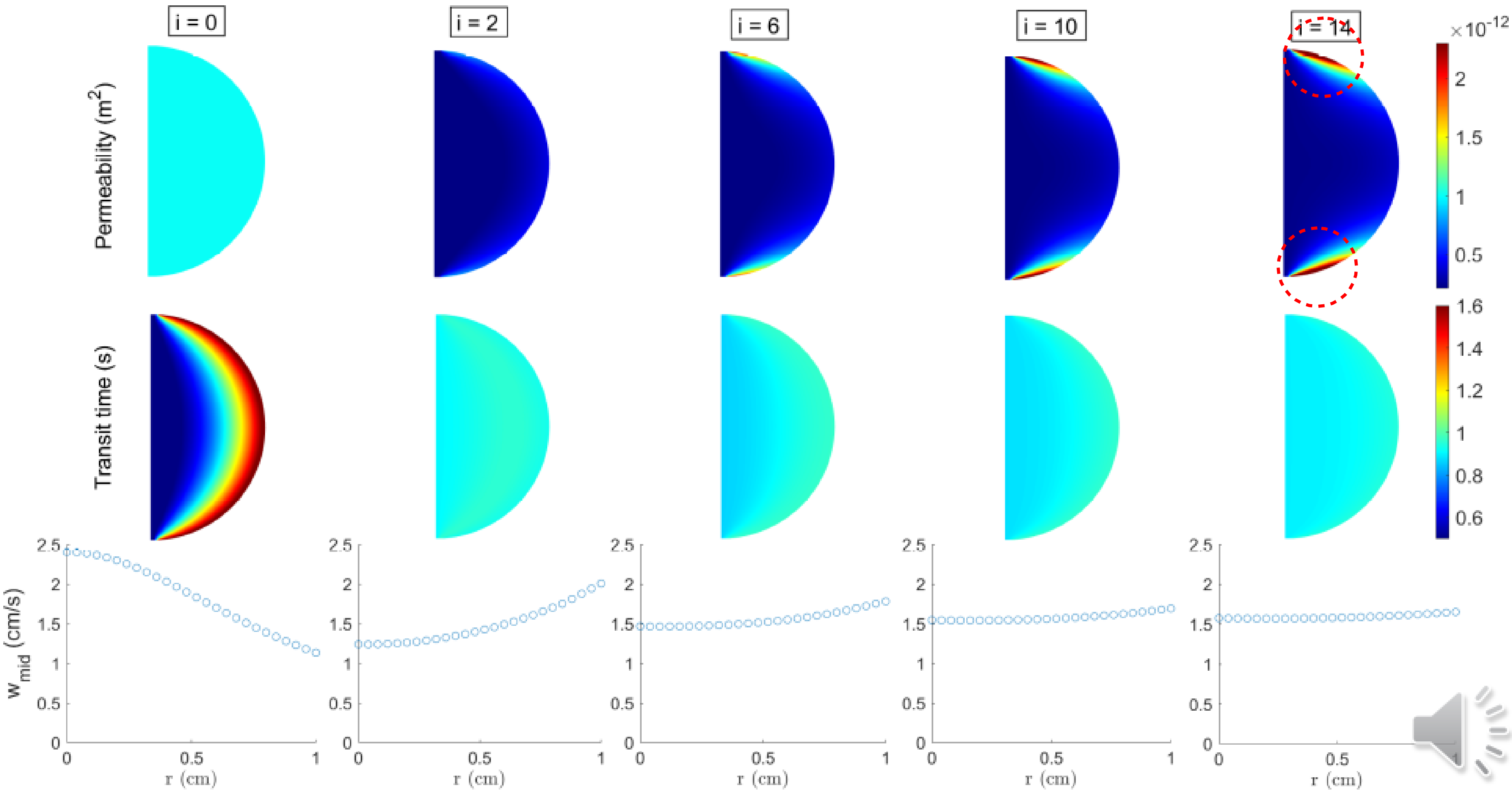
This algorithm adjusts the local value of the permeability according to the local value of the velocity and transit time.

Spherical Column with Graded Permeability

Non-Parametric Optimization Results

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

It is sufficient to grade the permeability near the sphere inlet and outlet



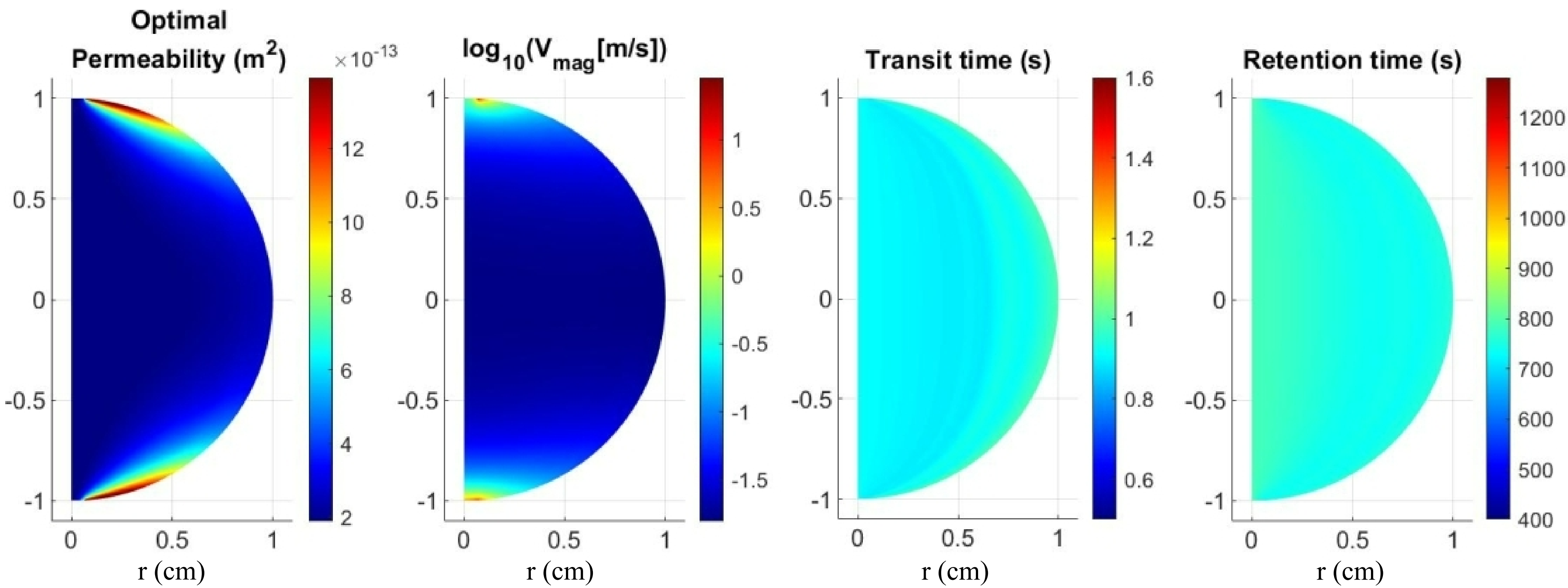
Spherical Column with Graded Permeability

Transit time vs. Retention time

The retention time is the time required for an analyte to travel to the outlet.

We assume that retention time is inversely proportional to porosity.

The porosity is related to the permeability by the Kozeny-Carman equation.



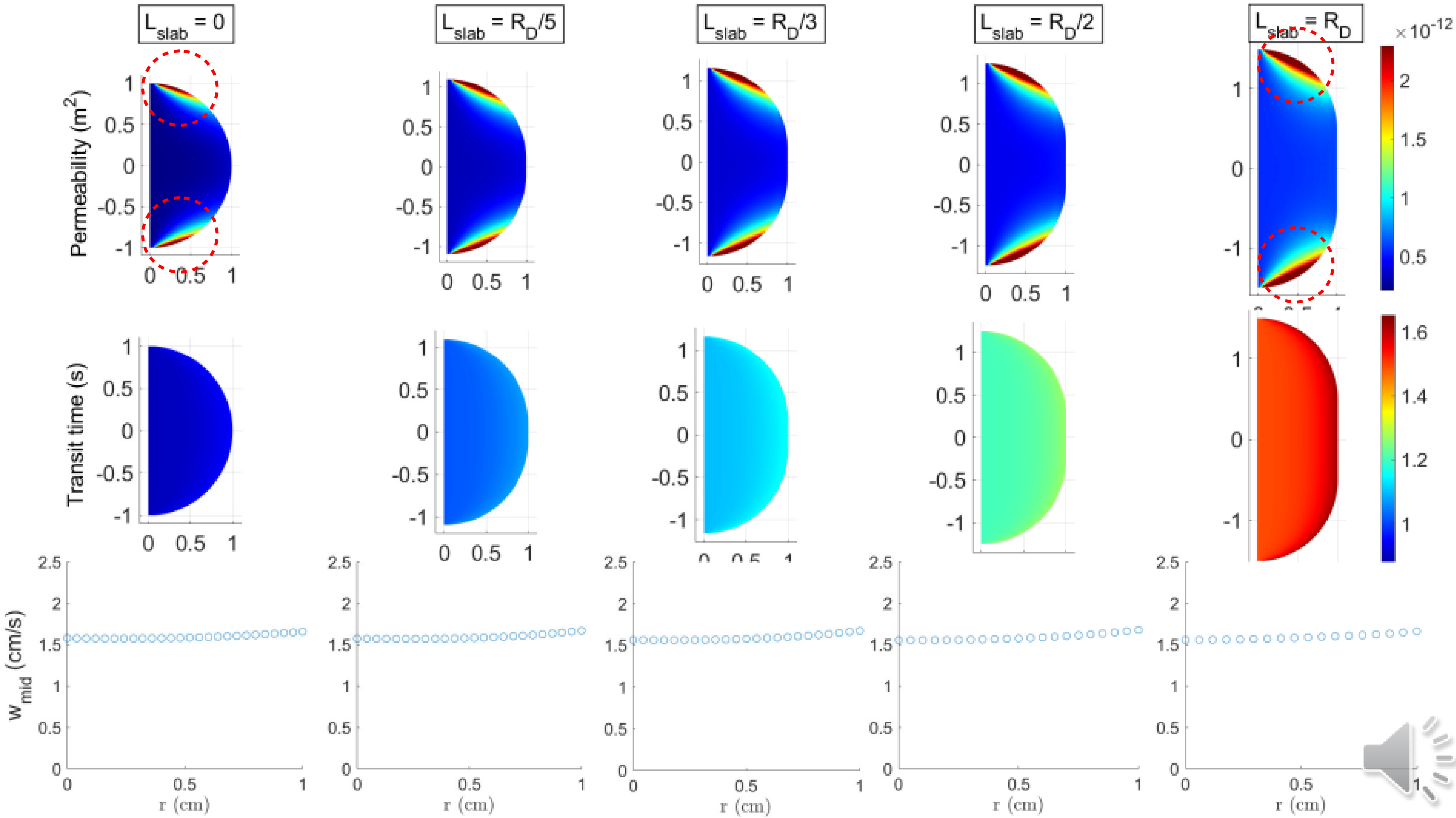
The optimal velocity is almost uniform in the radial direction

When we have optimized for uniform transit time, the retention time is also quite uniform, but slightly less so.

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. chromatography column)



Trust-region Newton method

Sandia has implemented more advanced optimization codes available that can efficiently accommodate a broader range of flow models and constraints.

Flow models implemented include Darcy's law and Stokes-Brinkman, allowing open channels to form.

T. Borrvall, J. Petersson. "Topology Optimization of Fluids in Stokes Flow." Int. J. Numer. Meth. Fluids 41, 77–107, 2003.

C. J. Lin and J. J. More. "Newton's Method for Large Bound-Constrained Optimization Problems." SIAM J Optim. 9 (4) 1100-1127, 1999.

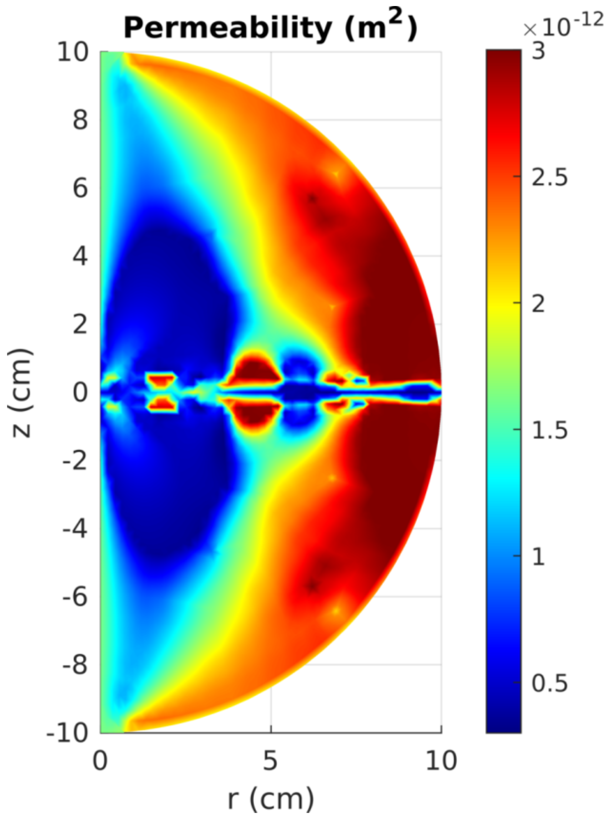
B. Jared et al. "Additive manufacturing: Toward holistic design." Scripta Materialia 125 141-147, 2017.

M. A. Heroux, R. A. Bartlett et al. "An overview of the Trilinos project." ACM Trans. Math. Softw. 31(3), 397-423, 2005.

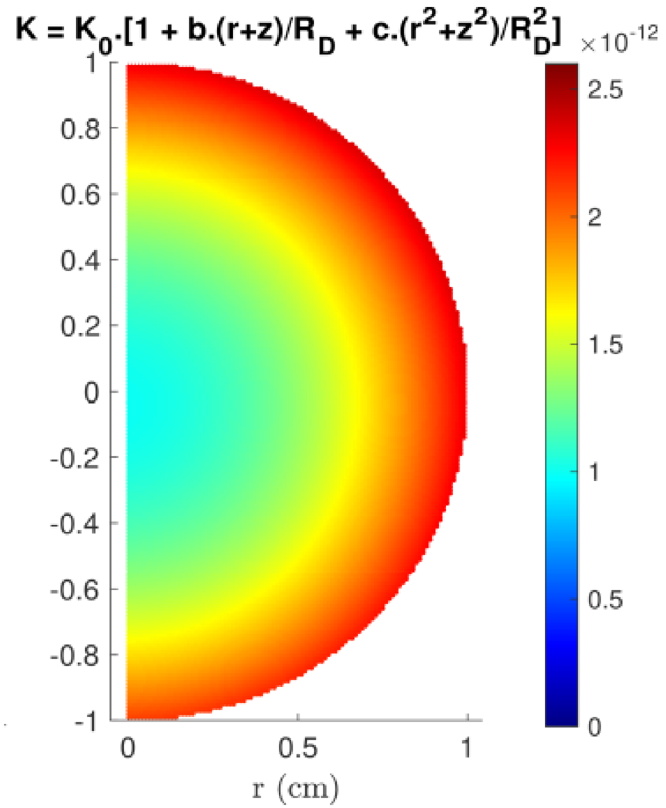
Spherical Column with Graded Permeability

Trust-region Newton method vs. Parametric

Trust-region Newton method produces a permeability field that is qualitatively similar to the one produces by parametric optimization, but with finer detail.



Trust-region Newton result for uniform midplane and axial velocity



Parametric optimization for uniform midplane velocity

Conclusions

Additive manufacturing techniques may enable novel architectures for porous media.

Optimized graded permeability can achieve uniform flow velocity, transit time, and/or retention time in porous devices.

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

Spherical columns with uniform transit or retention 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 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,
mnsallo@sandia.gov
www.sandia.gov/~mnsallo

Thank you for your attention!