Multiscale Modeling of Packed Beds

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Introduction and Motivation

What is it?

Modeling that resolves heat, mass, and momentum transport near catalyst surface (particle scale) and interstitial spaces (micro/meso scale) over a domain of 10-1000 catalyst particles in a packed bed.

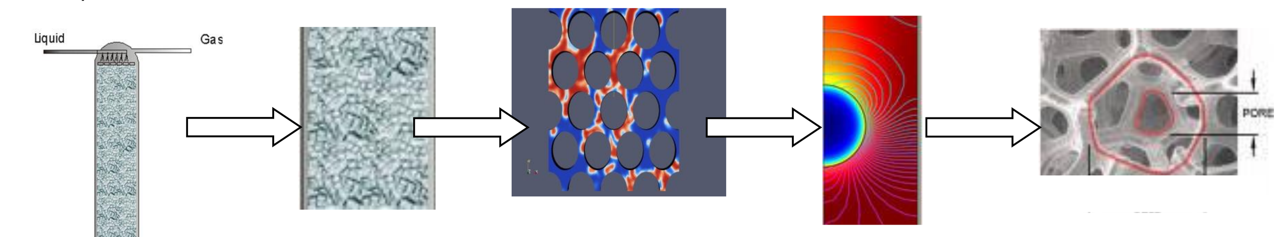


Figure1: Decreasing Length Scales In Trickle-Bed Reactors

Why is it important to study?

The geometry (intricate structure of the packed particles) influences phenomena within a packed bed across multiple length scales. On a reactor scale, bed geometry strongly influences overall pressure drop, residence time distribution, and dispersion of species. On the micro and particle scale, thin film flow, interphase mass transfer, local eddy formation, etc. are also strongly influenced by bed geometry.

Scope of Work

Domain Generation

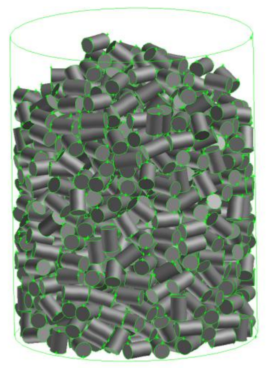
Generate a computational domain representing randomly arranged particles in a packed bed.

Model Development

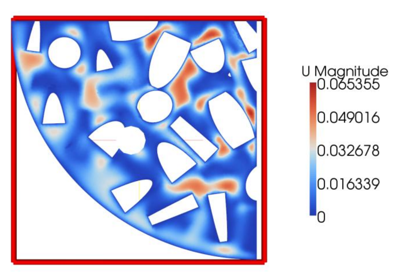
Use computational fluid dynamics to develop models describing heat, mass, and momentum transport in turbulent and laminar systems

Integration of Advanced Computing Technology

Utilize sparse linear system solvers on graphics processing units (GPUs) to increase speed of simulation



1000 Cylinders



Horizontal cross-section
Z-Velocity Profile

$$Ax = b$$

Domain Generation

The Monte-Carlo packing algorithm works by…

1. Approximating an initial condition of particles spread far apart in a very tall vertical tube.
2. Starting from the bottom of the tube, randomly rotate and translate each particle so that no particles overlap (time consuming step).
3. Decrease the height of the tube to further limit degrees of freedom.
4. As each packing cycle completes (i.e. each particle in the bed has been moved at least once), the overall porosity decreases to a steady state value.

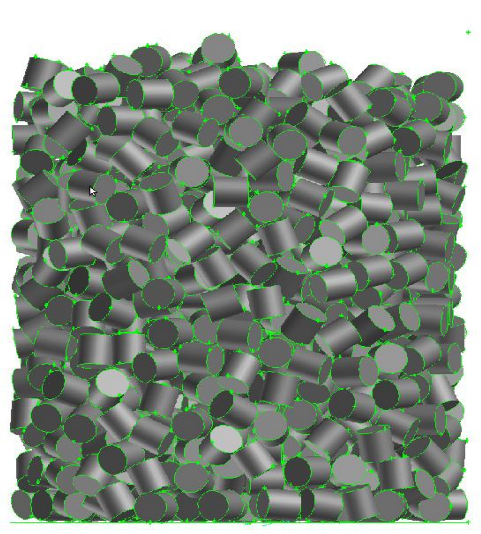
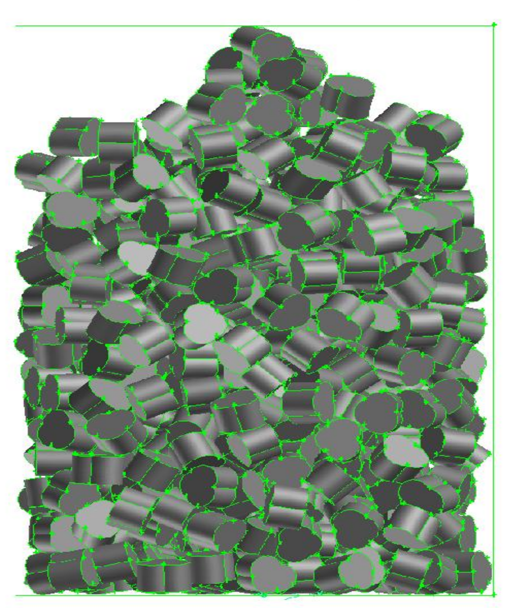


Figure 2: Packed bed domain for 1000 cylinders (left) and 250 trilobed (right) particles generated using developed algorithm



Domain Generation(Continued)

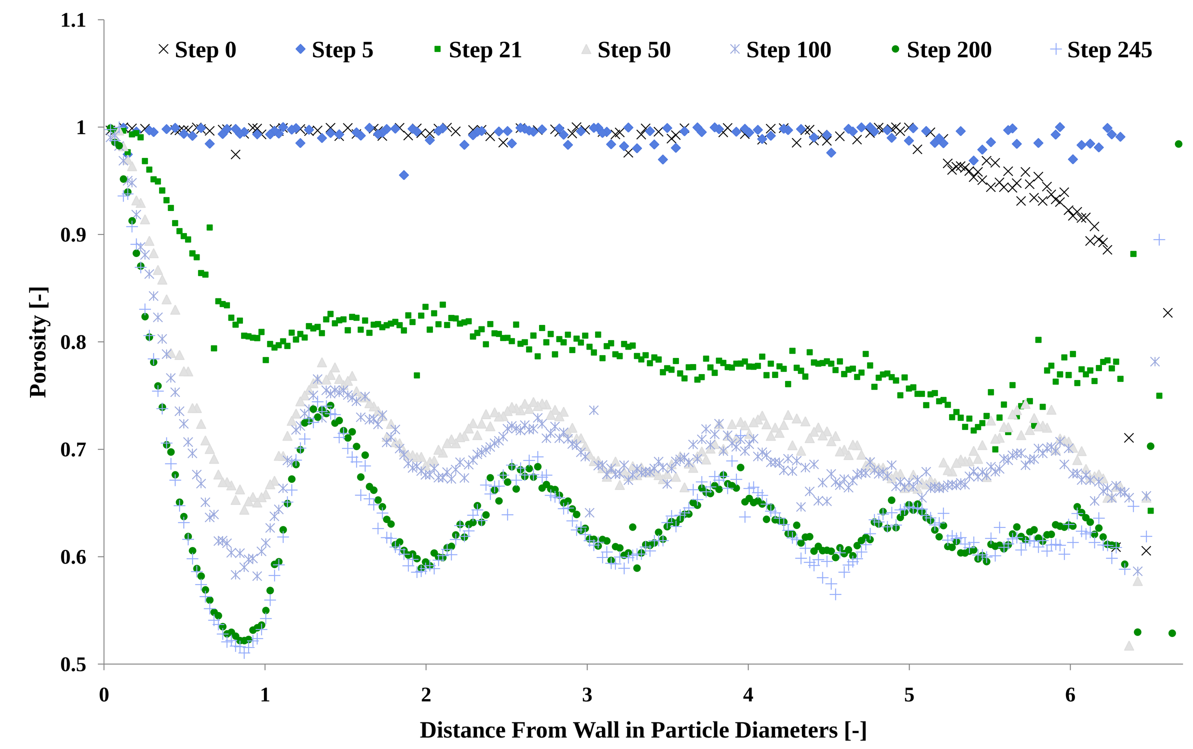


Figure 3: Time evolution of radial porosity distribution, showing increased packing and wall effect, seen similarly in previously published work in literature

Key Results:

- Algorithm produces domains with realistic bulk porosities (0.65)
- Radial porosity profiles are comparable to published experimental results.
- Trilobed and quadlobed particles can be packed with relative ease.
- Computational meshes for CFD modeling can be readily created.

Model Development and Simulation

Model Uses…

- Reynolds Averaged Navier-Stokes (RANS)-steady state solution
- Turbulent closure models
  - Spalart-Allmaras: One equation model
  - Launder-Sharma, Lam-Bremhorst, or Qzeta: Two equation low Reynolds number k-ε models
- No pressure closure models needed
- Meshes are on the order of 9 million cells (>36 million unknowns)

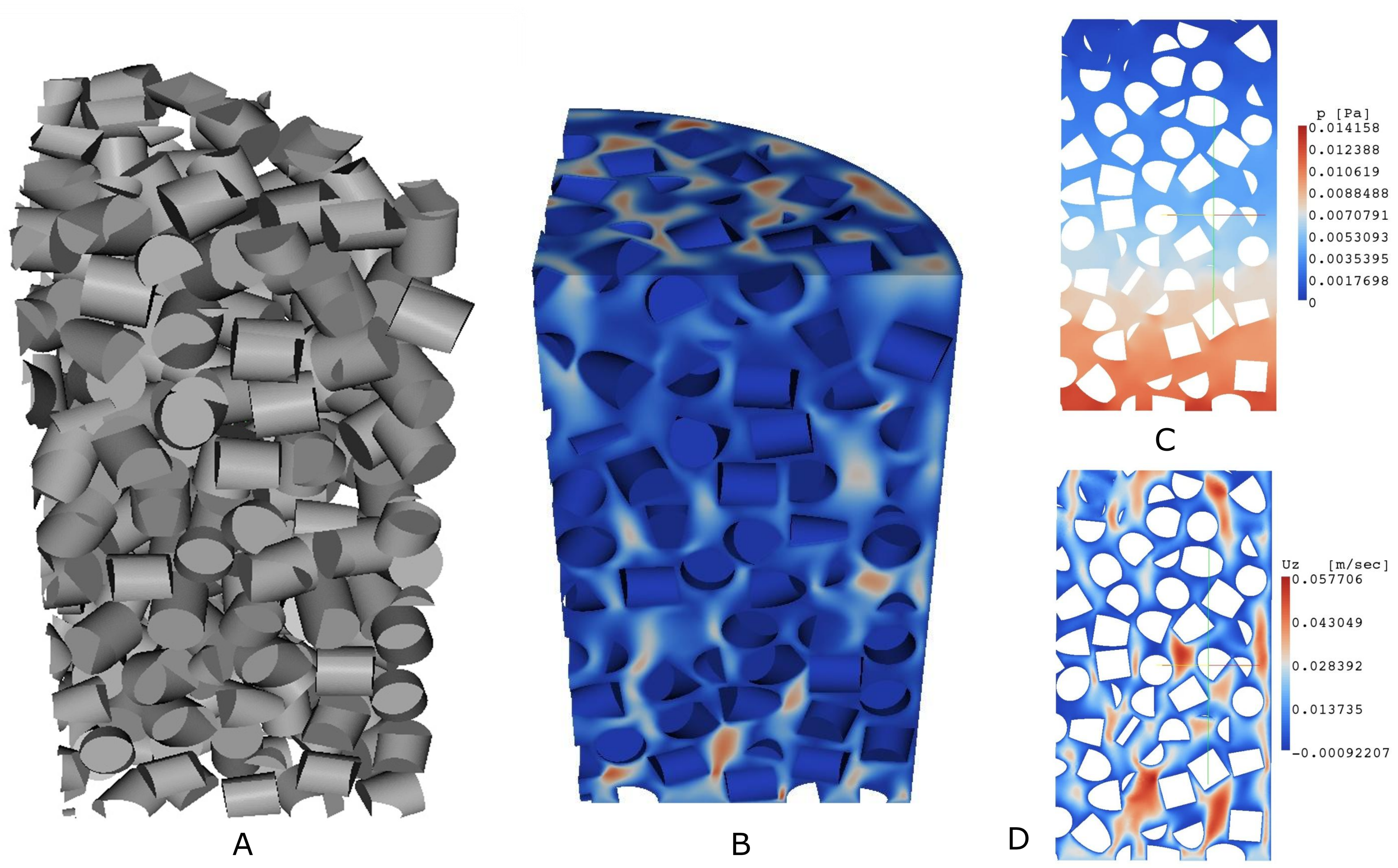


Figure 4: A) Computational domain of packed particles B) RANS solution showing velocity magnitude near edges of domain. C) View of pressure field in (-1 1 0) plane D) View of velocity magnitude in (-1 1 0) plane. Similar results can be shown for every variable in model.

Model Development and Simulation

Currently Moving Towards

RTD/Dispersion Studies

Unsteady RANS
- Determine best turbulence model
- Determine if inlet effects are significant
- Must worry about time scales of diffusion

LES/DES-LES
- Evaluate delta models and subgrid models
- Capture eddies that are smoothed by RANS and URANS

Key Results:

- Model correlates with Ergun's equation with amazing precision (E_1=190, E_2=0.468, R^2=0.99998 with 9 points)
- To capture influence of eddies, subgrid models or finer meshes must be used
- Time dependent models (URANS, LES, DES-LES) must be implemented to obtain dispersion coefficients for tracer injection

Advanced Hardware Integration

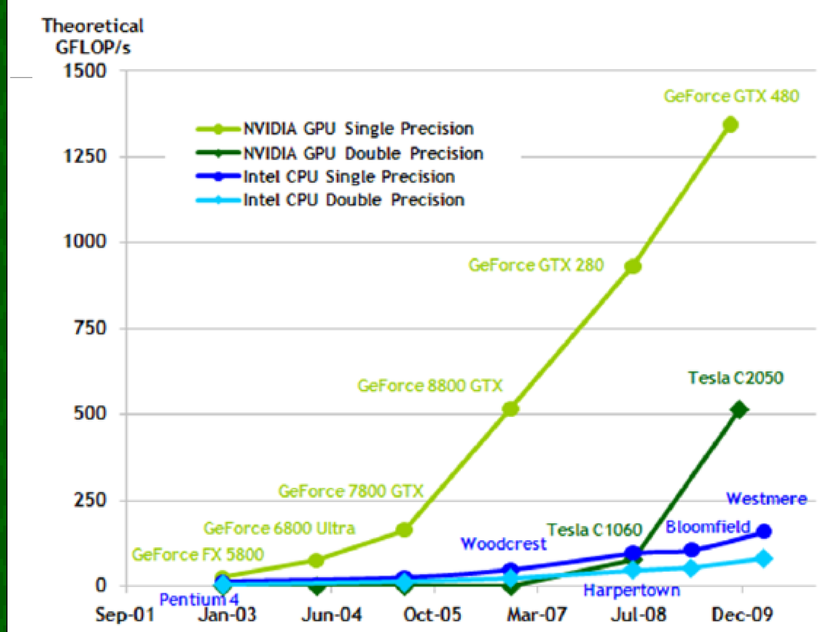


Figure 5: Comparison of single and double precision computations between Intel CPU and Nvidia GPU (Nvidia C Programming Guide, version 3.2. Nvidia Inc. 2010)

What is going on in CREL?

- GPUs have been integrated into OpenFOAM.
- 10X speedup of linear system solvers on meshes of several million cells.
- We are working with Nvidia to use larger, more powerful, GPUs (Tesla C2050) and run multiple GPUs in parallel

Pros

- Superior computational power over CPU (10X speedup of linear system solvers compared to equivalent OpenFOAM solver)
- More suited for Sparse matrix-vector operations than CPU
- Device-device memory bandwidth very fast

Cons

- Host-device memory transfer slow, only beneficial when large problems are solved
- For extremely large meshes, multiple GPUs must be used in parallel with communication using OpenMP

Conclusions and Take Home Message

✓An algorithm has been developed to create packed bed domains.

✓Generating a randomly packed domain is key to providing a realistic packed bed for industrially relevant simulations

✓Modeling pushes to show significance of interactions over multiple length and time scales .

✓To improve the understanding of the influence of small scale phenomena (turbulent eddies) on global parameters, one needs to implement DES or LES models.

✓Leveraging next generation computing technologies, such as GPUs, is key to solving extremely large problems.

References

D.P. Combest, P.A. Ramachandran, and M.P. Dudukovic. *Micro-Scale CFD Modeling of Trickle-Bed Reactors*. 2009-10 CREL annual Report. Pg 23-26, 2010.