Associate Professorship of Hydomechanics
TUM School of Design and Engineering
Technical University of Munich

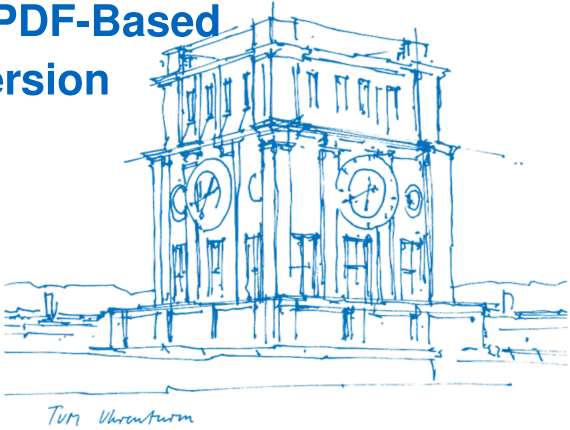
Investigation of a Velocity PDF-Based Model for Pore-Scale Dispersion

InterPore 2026

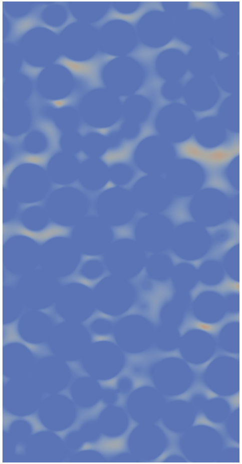
Yılkut Murat Aydın

Associate Professorship of Hydomechanics
TUM School of Design and Engineering
Technical University of Munich

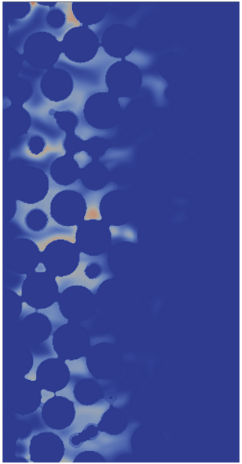
May 19th, 2026



Goal



Velocity field (Kooshapur)



Scalar field (Kooshapur)

- Non-Fickian scalar transport in porous media
- Transition behavior between non-Gaussian and Gaussian regimes
- Asymptotic limit of the effective diffusivity

Background Work and Extension

Meyer and Tchelepi, 2010

- Stochastic velocity PDF framework
- Macro-scale
- 2D heterogeneous log-conductivity fields
- Darcy equation

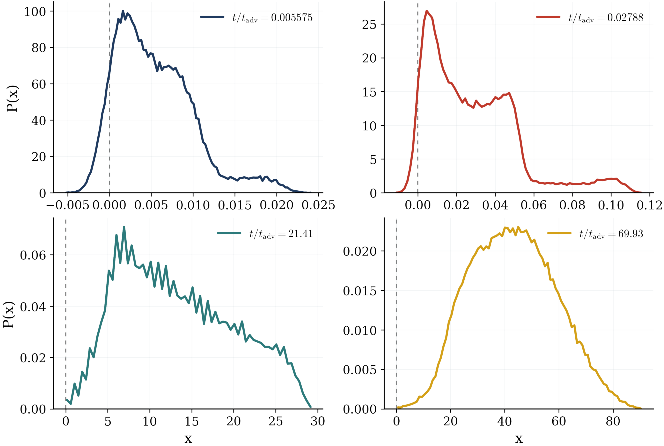
Kooshapur, 2016

- Stochastic velocity PDF framework
- Pore-scale
- 3D porous medium geometry
- DNS coupled with Eulerian scalar solver

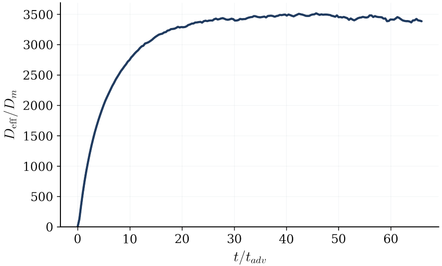
Current Work

- Peclet scaling
- Transition time-scales
- Possible improvements
- DNS coupled with Lagrangian solver

Why the velocity PDF?



Mean of the tracer cloud over time (BCC)



Effective diffusivity over time (BCC)

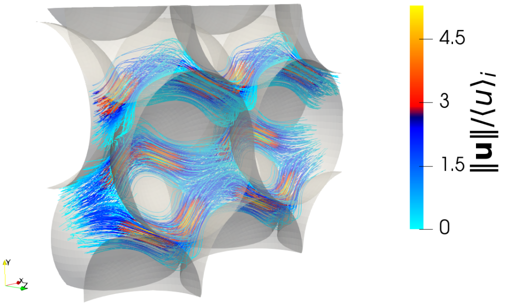
Our Dataset

Direct Numerical Simulations (DNS) (Manhart, 2004)

- **Flow regimes:** 3 laminar, 1 turbulent
- **Geometries:** FCC, BCC, and HCP pores
- **Resolution:** 160 and 320 cells per diameter

Massless Point Particle Tracking (Gollor, 2024)

- High Schmidt (Sc) numbers
- Peclet (Pe) number parameter space sweep
- Infinite domain for mass transfer



Flow pathlines through the pore geometry (HCP)

Model

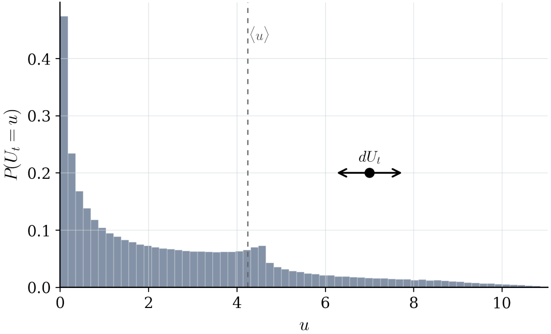
Advection-Diffusion in the physical space:

$$dX_t = U_t dt + \sqrt{2D_x} dW_t^{(x)} \quad (1)$$

Advection-Diffusion in the velocity space:

$$dU_t = A(U_t)dt + \sqrt{2D_u(U_t)} dW_t^{(u)} \quad (2)$$

$$\frac{\partial P(u)}{\partial t} = -\frac{\partial P(u)A(u)}{\partial u} + \frac{\partial^2 P(u)D_u(u)}{\partial u^2} \quad (3)$$



Velocity PDF (HCP)

Parameter Estimation

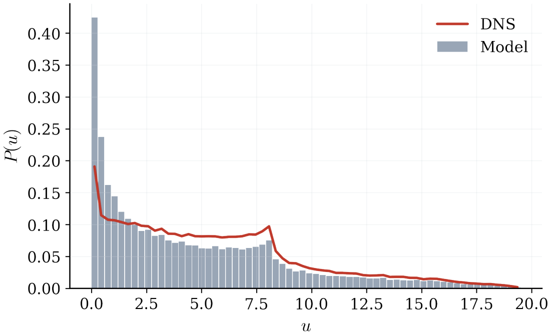
$$\cancelto{0}{\frac{\partial P(u)}{\partial t}} = -\frac{\partial P(u)A(u)}{\partial u} + \frac{\partial^2 P(u)D_u(u)}{\partial u^2}$$

Diffusion in the velocity space:

$$D_u(u) = \frac{\mathrm{Var}(d\tilde{U}_t | U_t = u)}{2dt} \quad (4)$$

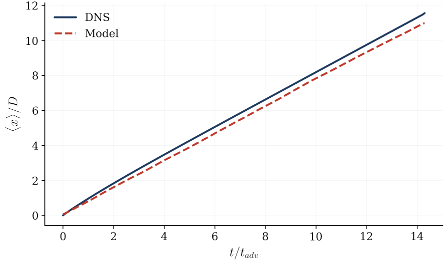
Drift in the velocity space:

$$A(u) = \frac{1}{2dtP(u)} \frac{\partial(\mathrm{Var}(d\tilde{U}_t | U_t = u)P(u))}{\partial u} \quad (5)$$

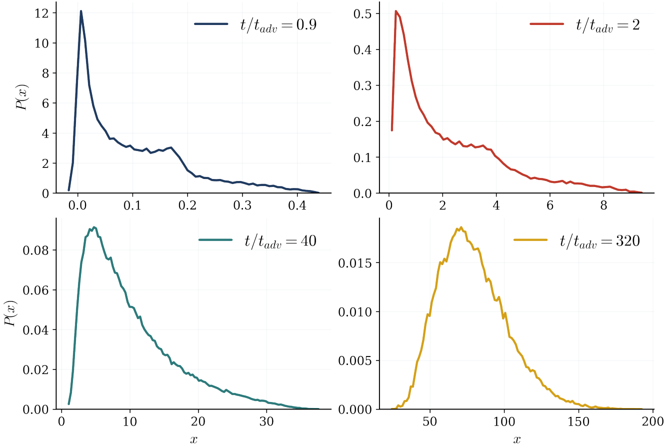


Velocity PDF (HCP)

Results

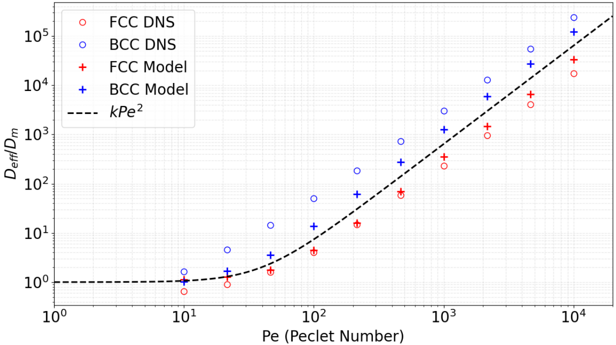


Mean of the tracer cloud over time (BCC)



PDFs of the tracer cloud over time (HCP)

Peclet Scaling



Comparison of model and the DNS values across Peclet numbers.

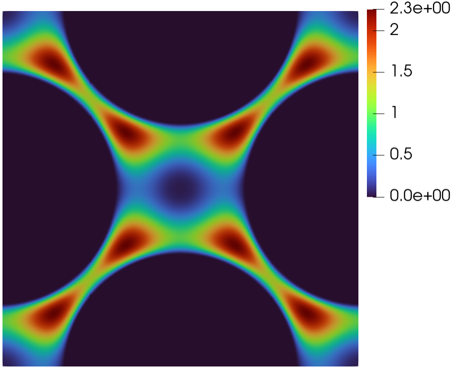
Fitting Equation:

$$f(Pe) = \epsilon + \beta \cdot Pe^{\gamma} \qquad (6)$$

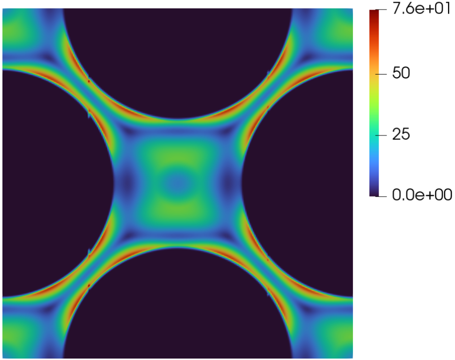
Calculated Coefficients

Case	ϵ	β	γ
BCC DNS	0.8968	0.0131	1.7920
FCC DNS	0.6477	0.0007	1.8417
BCC Model	1.1001	0.0013	2.0004
FCC Model	1.0202	0.0004	1.9808

State Aliasing - Markov Assumption



Streamwise velocity field $u/\langle u \rangle$



Velocity gradient magnitude field $|\nabla u|/\langle u \rangle$

Critical Assessment & Next Steps

Conclusions

- Accurate velocity PDF representation
- Accurate prediction of the mean
- Reduced computational load
- Qualitative prediction of the transition to the Gaussian state

Limitations

- Defaulting to the Taylor-Aris channel dispersion for Peclet scaling
- State aliasing in the lower velocity bins

Future Work

- Multiple Markov States
- Continuous Time Stepping Integration
- Deep Learning Methods

References

[1] Julius Gollor. *Implementation of a Lagrangian Particle Tracking Tool into the Numerical Flow Solver MGLET*. Tech. rep. Study Project Report, Associate Professorship of Hydromechanics. School of Engineering and Design, Technical University of Munich, 2024.

[2] Sheema Kooshpaur. “Modelling dispersion on the pore scale based on the velocity distribution function”. In: *PhD Thesis at TUM* -.- (2016), pp. –.

[3] Michael Manhart. “A zonal grid algorithm for DNS of turbulent boundary layers”. In: *Computers Fluids* 33.3 (2004), pp. 435–461. ISSN: 0045-7930.

[4] Daniel W Meyer and Hamdi A Tchelepi. “Particle-based transport model with Markovian velocity processes for tracer dispersion in highly heterogeneous porous media”. In: *Water Resources Research* 46.11 (2010).

Appendix - Derivation of the $d\tilde{U}_t$

$$dX_t = U_t dt + \sqrt{2D_x} dW_t^{(x)}$$

$$du = \frac{\partial u}{\partial x_i} dx_i + \frac{1}{2} \frac{\partial^2 u}{\partial x_i \partial x_j} dx_i dx_j + O(dx^3) \tag{7}$$

$$\begin{aligned} d\tilde{U}_t \approx \sqrt{2D_x} \frac{\partial u}{\partial x_i} dW_{it}^{(x)} + u_i \frac{\partial u}{\partial x_i} dt + D_x \frac{\partial^2 u}{\partial x_i \partial x_j} dW_{it}^{(x)} dW_{jt}^{(x)} \\ + \sqrt{2D_x} u_i \frac{\partial^2 u}{\partial x_i \partial x_j} dt \, dW_{it}^{(x)} + \frac{1}{2} u_i u_j \frac{\partial^2 u}{\partial x_i \partial x_j} dt^2 \end{aligned} \tag{8}$$