On the predictive capabilities of multiphase Darcy flow models

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Motivation
Multiphase flows in porous media

APPLICATIONS
Primary and secondary Oil Recovery, Groundwater remediation, Biological flows, Catalysis, Fluidized beds

Upscaled (effective, homogenized, averaged) transport models rely on physical and empirical parameters:

1. Absolute permeability (pure advection)
   \[ K \propto \frac{V}{\Delta P} \]

2. Dispersivity (diffusion + advection) \( D = D(V, D_m) \)

3. Relative permeability model
   \[ K_i = K_i(C) \propto \frac{V_i}{\Delta P_i} \]

4. Capillary pressure model \( P_i = P_i(P, C) \)

How to quantify the validity of the standard Darcy’s models?
How to check their actual predictivity?
**Pore-scale model**

Steady Navier Stokes equations in the pore space

\[ \nabla \cdot \mathbf{u} = 0 \quad \mathbf{u} \cdot \nabla \mathbf{u} = -\frac{1}{\rho} \nabla p + \frac{\mu}{\rho} \Delta \mathbf{u} \]

Advection Diffusion Reaction:

\[ \frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u} c + D_0 \nabla c) = 0 \]

**Darcy-scale model**

\[ \nabla \cdot \mathbf{V} = 0 \quad \mathbf{V} = -\frac{K}{\mu} \nabla P \]

Advection-Dispersion-Reaction:

\[ \frac{\partial C_\phi}{\partial t} + \nabla \cdot (\mathbf{V} C + D_\phi \nabla C) = 0 \]
Two phase immiscible flow

**Pore-scale model:**

\[
\frac{\partial}{\partial t} \rho + \nabla \cdot (\rho \mathbf{u}) = 0
\]

\[
\rho \frac{\partial}{\partial t} (\mathbf{u}) + \rho \mathbf{u} \cdot \nabla (\mathbf{u}) = -\nabla p + \mu \Delta \mathbf{u} + \kappa \sigma \mathbf{n} \delta(\Gamma)
\]

Interface advection:

\[
\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{u} c) = 0
\]

**Darcy-scale model**

Wang/Beckermann mixture model

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{V}) = 0 \quad \mathbf{V} = -\frac{\lambda(K_r)K}{\mu}(\nabla P - \rho \frac{\partial \mathbf{V}}{\partial t})
\]

Advection-Dispersion-Reaction (saturation equation):

\[
\frac{\partial C \phi}{\partial t} + \nabla \cdot [\mathbf{V}_c (K_r) C + D \phi \nabla C] = 0
\]
Outline

- Introduction, subsurface flow models
- UQ, pore-scale simulation and upscaling
- Model calibration and validation
- Conclusions
Bayesian UQ

In our predictions there exist many sources of error/uncertainty: numerics, model, randomness, parameters

\[
\pi(\theta|d) \propto \pi(d|\theta)\pi(\theta)
\]

\[
d = \mathcal{F}(\theta) + e
\]
**Heterogeneous and Multiscale Data Assimilation**

- Data come from Experiments at different scales
- Accurate physical models exist for pore-scale (Navier-Stokes) flow
- How to combine all these data?
- Development of stochastic models for upscaling and modelling errors

**Propagation Across Scales**

- Variability starts at the Navier-Stokes scale with random geometry
- It propagates to stochastic effective transport parameters of phenomenological or homogenized models
- With the help of spatial statistical model assumptions we can link to the macro-scale stochastic models

\(^a\) Random and periodic homogenization can be used only for global quantities with specific norms
Pore-scale (aka DNS)
Virtual validation data

Pore-scale simulation videos

+ Promising tool for model development, calibration and validation
- Still not fully predictive for complex flow problems due to numerical and geometrical approximations, sample size and physical assumptions

Pore-scale simulation of solute transport (Icardi et al, 2014)
Pore-scale simulation of CO$_2$ injection (Icardi et al, in preparation)
Monte Carlo and Multilevel MC

Given a random variable $X$ and a quantity of interest $Q$

$$E[Q(X)] = \frac{1}{M} \sum_{i=1}^{M} Q(X_i) + e \quad \text{with} \quad e \sim \mathcal{N}\left(0, \frac{Var(Q)}{M}\right)$$

**Multilevel Monte Carlo**

Giles, 2008

Given different accuracy levels $\ell$ and solution $Q^{(i)}_{\ell} = Q_{\ell}(X_i)$, the multilevel estimator is defined as

$$A_{ML} = \sum_{\ell=0}^{L} \sum_{i=1}^{M_{\ell}} \frac{Q^{(i)}_{\ell} - Q^{(i)}_{\ell-1}}{M_{\ell}}$$

with $M_{\ell}$ number of samples on level $\ell$ and $Q_{-1} = 0$.

- **Weak (mean) error:** $|E[Q - Q_{\ell}]| \approx 2^{-\alpha\ell}$
- **Multilevel variances:** $Var(Q_{\ell} - Q_{\ell-1}) \approx 2^{-\beta\ell}$
- **Computational work:** $E[\text{Cost}(Q_{\ell} - Q_{\ell-1})] \approx 2^{\gamma\ell}$
Improving MLMC

Hoel, Icardi, Tempone (in preparation)
Diffusion and Navier-Stokes equations in random perforated domains

**Multiscale MLMC**
- Using models at different scales via averaging/homogenization (e.g., Navier-Stokes/Darcy)
- Upscaled model should be fast \( \Rightarrow \) approximate/reduced model

**High-order MLMC**
- Differences with high-order stencils
- Richardson extrapolation for reducing bias (Giles, 2008; Lemaire, Pagés, 2013)
- Multi-Index Monte Carlo (MIMC, Haji-Ali, Nobile, Tempone, 2014)
- Weighted MLMC for reducing variance

\[ C_\ell Q_\ell - C_{\ell-1} Q_{\ell-1} + C_{\ell-2} Q_{\ell-2} \]

where \( C_i \) can be optimized to minimize the total variance of the estimator

These improvements are particularly important for complex black-box solvers when the convergence properties \((\alpha, \beta)\) are not guaranteed or non asymptotic
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Bayesian model validation

The validation pyramid
Calibration, Validation, Prediction

1. start with priors on unknown parameters
   \( \pi(\theta) \)
2. compute posterior \( \pi(\theta|d_c) \) given data \( d_c \) in the calibration scenario
3. forward propagation \( \pi(\theta|d_c) \) in a new validation scenario to obtain \( \pi(Q_c) \)
4. incorporate new data \( d_v \) and recompute \( \pi(\theta|d_c, d_v) \) and \( \pi(Q_d) \)
5. compute a "distance" \( \Delta \) (e.g., KL divergence) between \( \pi(Q_d) \) and \( \pi(Q_c) \)
6. if \( \Delta < TOL \) model is valid
7. prediction and forward propagation to obtain final QoI \( \pi(Q_v) \)

Ingredients: prior, data, error models
Strongly depends on: choice of measurements, choice of QoI

\(^1\)Babuska, Nobile, Tempone; Oden, Moser, Ghattas
Let us focus on a simple virtual experiment condition:

Pore-scale results are exact up to a small Gaussian uncorrelated error

One single sample

- Surfactant flooding experiment studied by Landry et al (2014)
- Low density and viscosity ratio ($\approx 1$)
- Quasi-neutral wetting (95 degrees contact angle)
- 5 imposed pressure gradients $10^3 – 10^7$ Pa/m
- Measured mean saturation in the volume
Models to calibrate

**Darcy-scale model**

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\]

Advection-Dispersion-Reaction (saturation equation):

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\frac{\partial C \phi}{\partial t} + \nabla \cdot \left[ \mathbf{V_c} (K_r) C + D \phi \nabla C \right] = 0
\]

- 1D Advection-Diffusion Equation

\[K_r = 1\]

\[\theta = \{K, D/\Delta P\}\]

- 1D ADE with Corey-Brook relative permeability

\[K_r \propto (1 - C)^\gamma\]

\[\theta = \{K, D/\Delta P, \gamma\}\]
**Implementation**

- Geometry (random packing): Blender + random packing code (Python)
- Pore-scale DNS: **OpenFOAM** (Algebraic VOF)

### 2-parameters model

- **Forward problem**: analytical solution of Advection-Diffusion in semi-infinite domain
- **Bayesian inversion**: **Chebfun** with full representation of 2D prior and posterior PDF
- **Resampling**: **Chebfun** to compute marginals and acceptance-rejection probabilities
- **Surrogate**: **Chebfun** (expensive)

### 3-parameters model

- **Forward problem**: **Chebfun** with **pde15s**
- **Bayesian inversion**: Matlab **MCMC** toolbox
- **Surrogate**: ??
Advection Dispersion Equation

Assimilation of single data sets
Advection Dispersion Equation
Assimilation of single data sets
Advection Dispersion Equation

Sequential assimilation of data sets 1 to 5
Advection Dispersion Equation

Sequential assimilation of data sets 2 to 4
Advection Dispersion Equation

Sequential assimilation of data sets 2 to 4
Brooks-Corey relative permeability

Second data set

![Graphs showing Log(D/ΔP) vs. Log(K) and Log(γ) vs. Log(K) with data points and fitted lines.](image)
Brooks-Corey relative permeability

Second + third data set
Brooks-Corey relative permeability

Second+third+fourth data set
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**ACHIEVEMENTS**

Usage of few global measurements and simple models for complex phenomena leads to:

- Surprisingly good fit of simple ADE for single data sets though with large uncertainties
- Improvement with relative permeability models but affected by overfitting

More efforts are needed for:

- Better error models and uncertainty for pore-scale data (ongoing)
- Adding wetting and higher-order (Forchheimer) terms to capture the whole range of flow rate (ongoing)

**FUTURE WORKS**

- Choose different validation and prediction scenarios
- Study influence of measurements and quantity of interest
- Modelling error for Darcy’s scale models
- Assimilate data computed on different samples
Research overview I

Multiphase flows simulation

Interphase tracking in unsaturated porous media

Drop impacts on random micro-surfaces

Adaptive Mesh Refinement, Numerical validation, Sensitivity to discretization parameters and convergence properties
Groundwater flows
Carbon storage and groundwater remediation

Pictures courtesy of IPCC (left) and Groundwater Engineering group at Politecnico di Torino (right)

Multi-scale models, stochastic PDEs, data assimilation, HPC implementation, Numerical and analytical upscaling (homogenization, volume averaging)
Random heterogeneous materials

Granular random packings, PDE discretisation in large complex geometry, Anomalous transport and mixing properties
Turbulent multiphase systems

Population balance for gas-liquid flows
Icardi, Ronco, Marchisio, Labois, 2014

Turbulence and LES, Nano-scale non-equilibrium fluids, Coagulation and transport of inertial particles, Micro-mixing models, Kinetic (Boltzmann, PDF) models
Mesoscale and kinetic models

Retain micro-scale and fluctuating properties through statistical description (Generalised Population Balance Model / Fokker-Planck)

\[ f(L; x, t) = \int_{\mathcal{R}^3} f(L, U_p; x, t) \, dU_p \]

**e.g., Particle Size Distribution**

\[ f(L; x, t) = \int_{\mathcal{R}^3} f(L, U_p; x, t) \, dU_p \]

\[
\text{St} = \frac{\tau_p}{\tau_f}
\]

Particles of different size behave very differently according to their Stokes number.
Example: particle-laden flow

Quadrature-based moment methods