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Dimensional effects on breakthrough behavior and pore-scale residence time distributions

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Abstract

Two-dimensional pore-scale models are widely used as computationally efficient alternatives to three-dimensional simulations. To assess the effects of this reduction in dimensionality, we use Lattice Boltzmann simulations to compare two dimensional (2D) and three dimensional (3D) permeability, breakthrough curves, and fluid age distributions for three types of porous media across a range of porosities. Permeability calculations show that 2D slices systematically underestimate the true (3D) permeability, with the magnitude of the discrepancy depending on pore geometry and being strongest at low porosity, indicating that out-of-plane connectivity drives the dimensional bias. Consistent with this, the pore-normalized Euler characteristic $\tilde{\chi}$, a topological measure of pore connectivity, largely tracks the 2D-vs-3D permeability difference across all three media and every porosity, pointing to its potential to indicate when 2D simulations may be suitable proxies for full 3D simulations. Dimensional effects on transport metrics show distinct medium-specific patterns. In the Fibrous porous medium, 2D-3D differences in mean travel time and breakthrough spreading stay almost constant across the explored permeability range. In the Gaussian medium, differences decrease with increasing permeability, while in the Overlapping Spheres medium, the 2D vs 3D differences in mean arrival time are larger and go in both directions, with no clear trend with permeability. Conservative and reactive tracers show similar breakthrough times and tracer spreading in 2D and 3D simulations. These results demonstrate that pore geometry and connectivity primarily govern dimensional bias with only smaller effects of tracer reactivity.

Article Highlights

- 2D pore-scale models systematically underpredict 3D permeability because of reduced connectivity.
- Dimensional bias in mean travel time and breakthrough spreading depends on pore structure and permeability.
- A geometry-only connectivity measure can indicate when a 2D model can stand in for a full 3D simulation.

Keywords Pore scale modeling, Dimensionality reduction, Permeability, Breakthrough curves, Residence time distribution

Mathematics Subject Classification (2020): 76S05 · 76M28 · 65Z05 · 55N31 · 86A05

1. Introduction

Solute transport in porous media controls a wide range of natural and engineered processes, including nutrient cycling, contaminant transport, enhanced oil recovery and carbon sequestration [1–3]. In the last decades, significant progress has been made in modeling these processes using simulations that explicitly represent the flow at the level of individual pores [4]. Pore-scale models describe non-Fickian transport behavior [5], long-tailed residence time distributions [6] and spatial heterogeneity in solute transport, which cannot be addressed by conventional Darcy-scale formulations [7]. Pore-scale simulations based on high-resolution micro-CT images have shown that pore architecture [6, 8] can result in solute spreading that is sensitive to connectivity between pores, and therefore dimensionality [9, 10]. Two-dimensional (2D) and three-dimensional (3D) porous media can exhibit fundamentally different flow and transport behaviors [11]. Early numerical work established that dimensionality directly controls flow connectivity and the resulting permeability [12] and that correct representation of pore geometry and connectivity leads to accurate estimation of transport properties [13]. In 2D, a significant fraction of pores do not contribute to the active flow pathways, particularly at low porosities, resulting in an effective porosity that is smaller than the nominal porosity, and in focused flow through narrow channels [14, 15], with a sharp decrease in permeability as porosity approaches the percolation threshold [16]. Hence, caution is warranted when extrapolating results from 2D analogues to a 3D porous medium, especially in settings where transport is governed by strong advection and intricate pore geometries [10, 17]. But while 3D simulations provide the most realistic representation of pore networks, they are computationally substantially more intensive. As a result, 2D domains derived from micro-CT slices or thin sections are still commonly used as proxies for 3D systems in modeling studies [8–10].

Differences in connectivity, tortuosity and mixing regimes between 2D and 3D pore structures may lead to inaccurate predictions of breakthrough curves or residence times [9–11, 17]. To

keep computational demand low while accounting for the absence of out-of-plane connections that alter flow pathways and connectivity relative to 3D [11], some studies match statistical properties such as porosity and two-point correlation functions between 2D and 3D representations of the same medium [8, 13, 17], rather than using observed 2D slices as the model domain. However, these low-order statistics may not fully capture pore connectivity and tortuosity, which govern flow and transport behavior [15] and direct comparisons between 2D and 3D domains have confirmed inconsistent flow predictions [11]. Alternatively, one may consider topological descriptors of the pore network, in particular the Betti numbers ($\beta_0, \beta_1, \beta_2$) and the Euler characteristic χ , which have been shown to correlate with permeability and capillary trapping in sandstones and other porous media [18, 19], motivating their use as easily computed measures for transport-relevant connectivity that only rely on information on the media structure.

Building on this body of work, this study explores the effect of dimensionality on solute transport behavior for different porous medium types, porosities and reactivity of the solute tracer. Using lattice Boltzmann simulations and statistical post-processing, we examine how dimensionality influences both solute breakthrough and fluid residence time distributions. We systematically explore (i) to what extent three-dimensional flow characteristics and medium properties can be predicted from two-dimensional simulations, (ii) how differences between two-dimensional and three-dimensional transport predictions vary with permeability and pore structure, and (iii) to what extent dimensional reduction affects conservative and reactive tracers differentially. For every 2D slice and its 3D parent we additionally compute the pore-normalized Euler characteristic $\tilde{\chi}$ and use it to test whether the dimensional discrepancy in permeability and transport metrics is explained by the connectivity that a flat slice cannot resolve.

2. Methods

2.1. Porous Media Generation

Computational domains of $100 \times 100 \times 100$ voxels were constructed for three different porous media types (Fibrous, Gaussian and Overlapping Spheres; see Fig. 1a for representative visualizations and Online Resource 2 for a discussion of the domain size), covering a wide range of industrial and environmental porous media. For each type, we designed 3D structures at low, medium and high porosities (0.4, 0.6 and 0.8, respectively). 2D domains were selected from the xz-planes whose pore geometry allowed for flow percolation (the imposed boundary conditions induce flow in the x-direction; see below).

Fibrous porous media, commonly representing biological tissues and engineered materials [20, 21], were generated by placing cylindrical fibers until a target porosity was reached. Each fiber

was assigned a fixed length (50 voxels) and a thickness (1 voxel for $\phi = 0.8$, 1.5 voxels for $\phi = 0.6$, and 2 voxels for $\phi = 0.4$) and placed by randomly selecting its starting point and direction. Voxels with centers within a fiber structure were assigned as solids.

Overlapping Spheres media were constructed to represent granular materials such as packed beds and sedimentary rocks [22, 23]. Spheres with a radius of 10 voxels were placed randomly and voxels with centers inside the spheres were set to solids. Spheres were added until the target porosity was met, resulting in approximately 300, 200 and 100 spheres for porosities of 0.4, 0.6 and 0.8, respectively.

Gaussian porous media exhibit pore distributions that resemble geological materials such as soil aggregates and sandstone rocks [24, 25]. A random number p between 0 and 1 was first assigned to each domain voxel. Then a Gaussian filter with a standard deviation of $\sigma = 2$ was applied to smooth this random field and produce features that covered roughly 5 voxels. Finally, a threshold value T was set to obtain the desired porosity by classifying voxels with $p > T$ as solids.

2.2. Pore-Scale Simulations

Fluid flow and mass transport processes were simulated with the Lattice Boltzmann (LB) Method resolving the Navier–Stokes (NS) and advection–diffusion–reaction (ADR) equations on a discrete voxel grid [26, 27]. Throughout this section, tilde notation ($\sim$) denotes dimensionless quantities, while parameters without tilde have metric units (e.g., dx in m, D in m^2/s), a full list of symbols used in this section, together with their names and units, is given in Table 1.

2.2.1. Fluid Flow

We implemented fluid flow using a three-dimensional lattice with 19 discrete velocity directions (D3Q19) [28], where the evolution of distribution functions follows the standard Lattice Boltzmann formulation [29]:

$$\tilde{f}_i(\tilde{r} + \tilde{c}_i \Delta \tilde{t}, \tilde{t} + \Delta \tilde{t}) = \tilde{f}_i(\tilde{r}, \tilde{t}) - \frac{\Delta \tilde{t}}{\tilde{\tau}} [\tilde{f}_i(\tilde{r}, \tilde{t}) - \tilde{f}_i^{eq}(\tilde{r}, \tilde{t})] \quad (1)$$

where $\tilde{f}_i(\tilde{r}, \tilde{t})$ represents the particle distribution function along direction i at position $\tilde{r}$ and time $\tilde{t}$, $\tilde{c}_i$ is the lattice velocity and $\tilde{\tau}$ is the relaxation time controlling fluid viscosity and the last term on the right-hand side represents the Bhatnagar Gross Krook (BGK) operator. The equilibrium distribution function $\tilde{f}_i^{eq}$ is defined as [29]:

$$\tilde{f}_i^{eq} = \tilde{\omega}_i \tilde{\rho} \left[1 + \frac{\tilde{u} \cdot \tilde{c}_i}{\tilde{c}_{s,NS}^2} + \frac{(\tilde{u} \cdot \tilde{c}_i)^2}{4\tilde{c}_{s,NS}^4} - \frac{\tilde{u} \cdot \tilde{u}}{2\tilde{c}_{s,NS}^2} \right] \quad (2)$$

where $\tilde{\omega}_i$ are the lattice weights specific to the D3Q19 model, $\tilde{\rho}$ is the local fluid density ($\tilde{\rho} = \sum \tilde{f}_i$), $\tilde{u}$ is the macroscopic velocity $\tilde{\rho}\tilde{u} = \sum \tilde{c}_i\tilde{f}_i$ and $\tilde{c}_{s,NS} = \frac{1}{\sqrt{3}}$ is the D3Q19 lattice speed of sound [30].

The lattice kinematic viscosity was determined from the relaxation time as $\tilde{\nu}_{NS} = \tilde{c}_{s,NS}^2(\tilde{\tau}_{NS} - 0.5)$, where $\tilde{\tau}_{NS}$ is the dimensionless relaxation time that controls the rate of collision toward equilibrium.

Table 1. Nomenclature. Every symbol used in the pore-scale modelling framework of section 2.2, listed with its meaning and physical units. Dimensionless lattice-Boltzmann quantities carry a tilde ($\sim$); all other quantities are in SI units.

Symbol	Meaning	Units
dx	grid spacing (voxel edge length)	m
dt	physical time step	s
D	diffusion coefficient	$\text{m}^2 \text{s}^{-1}$
ν	kinematic viscosity	$\text{m}^2 \text{s}^{-1}$
L	domain length	m
ΔP	pressure drop across the domain	Pa
k	permeability	m^2
U	Darcy velocity	m s^{-1}
Pe	Péclet number	dimensionless
Da_1	first Damköhler number	dimensionless
R	reaction rate	s^{-1}
C	solute concentration	mol m^{-3}
φ	porosity	dimensionless
$\tilde{\chi}$	pore-normalized Euler characteristic	dimensionless
$\beta_o, \beta_l, \beta_z$	Betti numbers (bodies, loops, pockets)	dimensionless
$\tilde{f}_i$	particle distribution function (LB)	dimensionless
$\tilde{c}_i$	lattice velocity (LB)	dimensionless
$\tilde{\tau}_{NS}, \tilde{\tau}_{ADE}$	LB relaxation times (flow, transport)	dimensionless
$\tilde{\nu}, \tilde{D}$	lattice kinematic viscosity, lattice diffusivity	dimensionless
$\tilde{c}_s$	lattice speed of sound	dimensionless

Starting with an initial guess of the pressure drop $\tilde{\Delta P}_0$ between inlet and outlet, the flow field was calculated and the permeability ($\tilde{k}$) was estimated using Darcy's law: $\tilde{k} = \frac{(\tilde{u}_0 \times \tilde{\nu}_{NS} \times \tilde{L})}{\tilde{\Delta P}_0}$,

where $\tilde{u}_0$ is the Darcy velocity measured in this initial run, $\tilde{\nu}_{NS}$ is the kinematic viscosity, and $\tilde{L}$ is the domain length (all in lattice units). Holding the Péclet number ($\tilde{Pe}$) constant, and with a given $\tilde{D}$ and $\tilde{L}$, the target Darcy velocity is $\tilde{u}_{target} = \frac{(\tilde{Pe} \times \tilde{D})}{\tilde{L}}$. Substituting this expression into Darcy's law yields the corrected pressure drop across the domain: $\tilde{\Delta P}_{new} = \frac{\tilde{u}_{target} \times \tilde{\nu}_{NS} \times \tilde{L}}{\tilde{k}}$, which was used in the next Navier–Stokes simulation and repeated until convergence. No-flow boundaries were imposed along the lateral domain boundaries and no-slip conditions at the solid–fluid interfaces were enforced using the bounce-back scheme [31].

The physical time step Δt (in seconds) was calculated as:

$$\Delta t = \frac{(\tilde{D} \times dx^2)}{D} \quad (3)$$

where $\tilde{D}$ is the lattice diffusivity (dimensionless), dx is the grid spacing (m), and D is the aqueous diffusion coefficient ($m^2 \cdot s^{-1}$). For a detailed description of the pore scale modeling environment see [32].

2.2.2. Mass Transport

To simulate mass transport, we used a D3Q7 lattice that approximates the advection-diffusion equation [33]:

$$\tilde{g}_i^j(\tilde{r} + \tilde{c}_i \Delta \tilde{t}, \tilde{t} + \Delta \tilde{t}) = \tilde{g}_i^j(\tilde{r}, \tilde{t}) - \frac{\Delta \tilde{t}}{\tilde{\tau}_g^j} [\tilde{g}_i^j(\tilde{r}, \tilde{t}) - \tilde{g}_i^{j\,eq}(\tilde{r}, \tilde{t})] + \tilde{\Omega}_t^{RXN}(\tilde{r}, \tilde{t}) \quad (4)$$

with the equilibrium distribution function:

$$\tilde{g}_i^{j\,eq}(\tilde{r}, \tilde{t}) = \tilde{\omega}_i \tilde{C}_j \left[1 + \frac{\tilde{u} \cdot \tilde{c}_i}{\tilde{c}_{s, ADE}^2} \right] \quad (5)$$

where $\tilde{\tau}_g^j$ is the mass transport relaxation time, $\tilde{C}_j$ represents the concentration of solute j , $\tilde{\omega}_i$ are the D3Q7 lattice weights ($\tilde{\omega}_0 = \frac{1}{4}$ for the central node, $\tilde{\omega}_{1-6} = \frac{1}{8}$ for adjacent directions) and $\tilde{c}_{s, ADE}^2 = 1/4$ for the D3Q7 lattice, yielding a lattice diffusivity of $\tilde{D} = \tilde{c}_{s, ADE}^2 (\tilde{\tau}_{ADE} - 0.5)$ [34].

Rather than computing the reaction term in the collision step ($\tilde{\Omega}_t^{RXN}$ in Eq. 4), we utilize operator splitting and compute transport using the lattice Boltzmann method and then update solute concentrations based on the reaction rates R_j , which for each time step (Δt) are calculated from the local concentrations and user-defined rate expressions:

$$C_j^{t+1} = C_j^t + R_j^t \Delta t \quad (6)$$

To quantify how solutes migrate through the porous medium, we performed conservative and reactive tracer simulations. For conservative tracers, unit concentration was imposed at the inlet boundary ($C_0 = 1$), while a zero-gradient (Neumann) condition was applied at the outlet. Grain surfaces and domain sides were treated with no-flux (bounce-back) boundary conditions and the initial concentration throughout the domain was set to zero. For reactive tracers, the concentration at the inlet boundary as well as the initial concentration were set to 0 and the reaction rate is set to unity, such that the tracer concentration corresponds to the fluid age [35, 36].

The simulations were run under advection-dominated settings ($Pe = 4.1, 12.5$ and 37.5 , achieved by imposing a diffusion coefficient of $10^{-13} \text{ m}^2 \text{ s}^{-1}$); the reactive tracer simulations represent Damköhler numbers ($Da_1 = \frac{R L^2}{Pe D}$) $\gg 1$ in all our settings.

2.3. Pore-Network Topology

To quantify pore-network connectivity from the binary geometry alone we use persistent homology [37]. For each medium we compute three Betti numbers from the signed Euclidean distance field of the pore phase: β_0 counts the number of separate pore bodies, β_1 counts closed loops in the pore network, and β_2 counts grain pockets fully enclosed by pore (β_2 is structurally zero in 2D because a flat image cannot enclose a pocket). The three counts combine into the Euler characteristic $\chi = \beta_0 - \beta_1 + \beta_2$. To compare 2D slices to 3D cubes on the same scale we divide χ by N_p , the pore-voxel count of the domain to compute the pore-normalized Euler characteristic $\tilde{\chi} = \frac{\chi}{N_p}$. Negative $\tilde{\chi}$ identifies a well-connected pore network dominated by loops; positive $\tilde{\chi}$ identifies a fragmented pore network. The signed Euclidean distance, the persistent-homology computation and the per-realization values of $\tilde{\chi}$ are described in Online Resource 1 (Sect. A.2 for the methods, Tables A3 and A4 for the per-medium counts).

3. Results and Discussion

3.1. Flow Structure and Tracer Patterns

Visualizations of the simulations qualitatively show the importance of the porous medium structure (Fig. 1a) for the heterogeneity in flow (Fig. 1b) and tracer (Fig. 1c) fields. In the Fibrous medium, there are clear preferential flow paths which are produced by the continuous high-velocity channels (green/yellow areas) that run along the fiber directions (Fig. 1b, left). In the Overlapping Spheres medium, the velocity field is characterized by a combination of dispersed low-velocity regions and distinct high-velocity channels along interconnected pores, including the prominent flow pathway visible in Fig. 1b (right). In the Gaussian medium, we observe many small and scattered regions of fast flow (green and yellow zones) surrounded by much larger

areas of slow flow (dark blue) which results in a spatially complex and branching flow field (Fig. 1b, middle).

In conservative tracer simulations (Fig. 1c), high-concentration tracer regions (red) are located on the left side of the porous medium with a gradual transition to lower concentrations toward the right side (blue colors near the outlet), showing that the tracer propagates largely along the main flow direction. In the Overlapping Spheres medium, the tracer distribution is less uniform with pronounced concentration gradients extending both along and perpendicular to the main flow direction, reflecting the preferential flow paths seen in Fig. 1b (right). In the Gaussian medium, the tracer penetrates only a small distance into the domain, with a sharp front near the inlet boundary (Fig. 1c, middle). Downstream, concentrations drop to intermediate levels (green/yellow) and then transition to low concentrations (blue), reflecting the low permeability of this medium compared to the Fibrous and Overlapping Spheres domains (Fig. 1c).

The fluid age distributions reveal differences in residence time distributions between porous media (Fig. 1d). In the Fibrous medium the age field is layered and directionally aligned with the flow, while we observed more irregular and locally variable age patterns in the Gaussian and Overlapping Spheres domains (Fig. 1d). These variations show how pore geometry creates poorly connected regions characterized by long residence times.

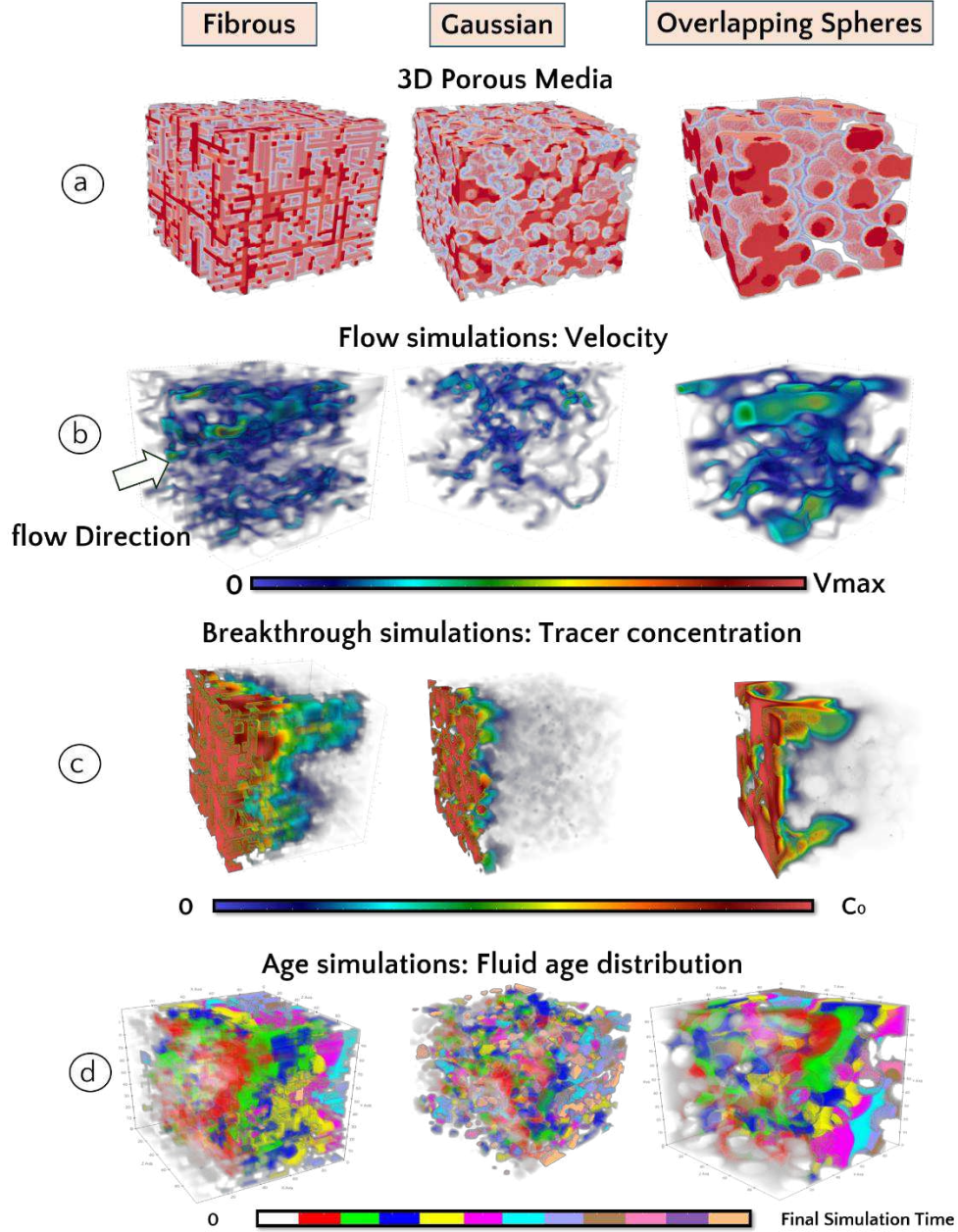


Fig. 1 Representative visualization of the three 3D porous media (Fibrous, Gaussian and Overlapping Spheres) at porosity $\phi = 0.4$ and intermediate Péclet number ($Pe \approx 12.5$), showing (a) pore geometry, (b) velocity magnitude, (c) conservative solute concentration, and (d) fluid age at $t = 810$ s

3.2. Permeability

Comparison of results from 3D simulations to those from 2D slices extracted from the 3D medium shows that 2D simulations generally underestimate permeability across all media types (compare the 2D-slice markers with the 3D star markers in Fig. 2). The differences vary with both the porous medium type and porosity, with discrepancies between 2D and 3D

permeability estimates decreasing as porosity increases. The permeabilities computed for 2D slices in the Fibrous medium were nearly 10 times lower than 3D-based values at low porosity ($\phi = 0.4$). The Gaussian medium shows smaller differences, with 2D values roughly four times lower at low porosity. The difference was also large for the Overlapping Spheres medium for one of the three 2D slices at low porosity, yet this medium exhibits the smallest dimensional discrepancy overall.

Individual 2D slices may not exhibit the same porosity as the entire 3D domain. To account for the effect of porosity differences, we used the Kozeny–Carman relationship to estimate the permeability as a function of porosity for both 2D and 3D simulation results. Our findings indicate that the permeability values based on the Kozeny–Carman relationship for 2D slices also fall below those of 3D results (compare solid and dashed lines in Fig. 2), indicating that porosity differences do not explain the observed dimensional discrepancies. This is in line with findings by [11] who showed that flow fields in 2D lack the spatial variability and connectivity observed in 3D systems.

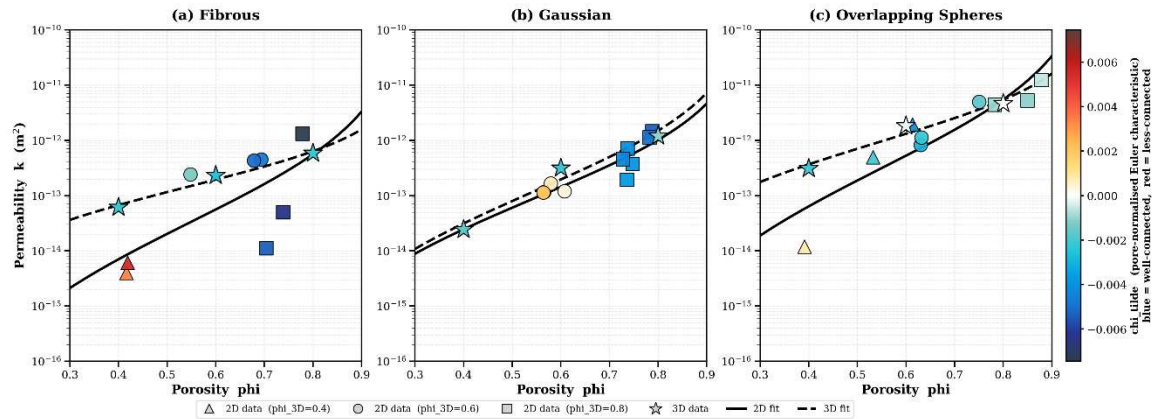


Fig. 2 Permeability versus porosity per medium, with each marker colored by the pore-normalized Euler characteristic $\tilde{\chi}$, a topological descriptor of pore-network connectivity. Three panels split the data by medium: (a) Fibrous, (b) Gaussian, (c) Overlapping Spheres. The x axis is porosity ϕ ; the y axis is permeability k in m^2 on a log scale. Stars mark the 3D cubes. Markers for 2D slices are grouped by the porosity of the 3D parent they were extracted from: triangles for $\phi(3D) = 0.4$, circles for $\phi(3D) = 0.6$, and squares for $\phi(3D) = 0.8$. Marker color follows a blue-to-red color bar (blue = negative $\tilde{\chi}$, well-connected pore network dominated by loops; red = positive $\tilde{\chi}$, fragmented pore network). The solid black curve in each panel is a Kozeny–Carman fit to the 2D points; the dashed black curve is the same fit to the 3D points

The marker colors in Fig. 2 link permeability to pore-network connectivity. Orange and red markers (positive $\tilde{\chi}$, poorly connected pore networks) appear mostly at the lower

permeabilities, whereas blue markers (negative $\tilde{\chi}$, well-connected networks) cluster at the higher permeabilities. The 2D–3D contrast in $\tilde{\chi}$ is largest in the Fibrous (a) and Gaussian (b) media and remains near zero in the Overlapping Spheres medium (c). In general, the 2D and 3D permeabilities diverge where their $\tilde{\chi}$ values diverge, but not always: at $\phi = 0.8$ in the Fibrous medium and at $\phi = 0.6$ in the Gaussian medium, the 2D and 3D permeabilities are similar even though $\tilde{\chi}$ differs. $\tilde{\chi}$ is therefore an inexpensive, geometry-only proxy for connectivity, but only a partial predictor of 2D-vs-3D permeability differences (Fig. A12). As in our dimensional comparison, the porosity of the 2D slices differ from that of the parent 3D domain, we accounted for the effect of the porosity difference between them by correcting the computed 2D permeability for the porosity offset, using the medium's 2D Kozeny-Carman curve (see Online Resource A3.3), so that the residual 2D vs 3D permeability mismatch reflects the topology difference alone (Fig. A13). This reinforces the general pattern suggesting that the pore-normalized Euler characteristic predicts the direction of the dimensional gap (more so than its magnitude).

The underestimation of the true permeability from 2D slices occurs because dimensional reduction modifies pore connectivity and the geometry of flow paths [38, 39]. Previous research [16] has shown that effective porosity, the fraction of pore space substantially involved in transport, can be significantly less than total porosity in two-dimensional systems, disrupting the continuity of the flow network. At low porosities, there is a significant increase in tortuosity, which forces fluids to follow longer and more complex pathways [38, 40]. The observed effects align with our model results, in which the differences between 2D and 3D are most significant at low porosities. This is also consistent with previous studies [41, 42] showing that low-porosity rocks tend to be less connected in 3D as well and a 2D slice cut from such a medium loses the few remaining out-of-plane routes, pushing the 2D permeability further below the 3D value.

3.3. Transport Metrics across the Permeability Spectrum

After confirming that porosity differences between 2D and 3D simulations do not explain the observed differences in permeability, we explored whether 2D models systematically and predictively deviate from their 3D equivalents, and to what extent dimensionality affects conservative and reactive tracers differently across pore structures. To that end, we computed the relative differences between 2D and 3D results for each porous medium. We calculated breakthrough curves for both conservative and reactive tracers under similar flow conditions to directly compare their behavior across dimensions. Flux-weighted breakthrough curves for all porous media, porosities and Péclet numbers are shown in Fig. C1 of Online Resource 3. From each breakthrough curve, we derived two key measurements: the first temporal moment (M_1),

which represents the mean tracer arrival time, and the coefficient of variation (CV), which represents the dispersion of the breakthrough (Online Resource 3).

3.3.1 Dimensional Differences in Transport Metrics Across Porous Media

The relative differences between 2D and 3D transport indicators (M_1 and CV) show medium-dependent trends with permeability (Fig. 3). In each panel, the y-axis is the relative 2D–3D difference: a value of zero means the 2D and 3D simulations agree, and deviation from zero measures how far the 2D result diverges from the 3D one (positive = 2D overestimates, negative = 2D underestimates). In the Fibrous medium, M_1 and CV are typically larger for 2D than 3D simulations (Figs. 3a, d), with the relative 2D–3D difference in M_1 and CV remaining almost constant throughout the entire permeability range (regression slope is close to zero; Table C1, Online Resource 3). This similarity across a wide range of permeabilities may occur because flow in the Fibrous medium tends to organize into a few dominant channels, so more of the tracer follows the same main routes rather than spreading through a tangled network of pores [43].

In the Gaussian medium, the relative differences of M_1 and CV of 2D and 3D both show negative slopes (Fig. 3b, e). This is most pronounced for CV (regression slope of the relative difference in CV vs. $\log_{10}k = -0.25 \pm 0.07$; Fig. 3e), with the 2D–3D differences becoming smaller as permeability increases. This is indicative of low-permeability domains that contain narrow throats that restrict flow in 2D but can be bypassed through out of plane routes in 3D, which can give 3D simulations faster or broader breakthrough behavior [44, 45]. As permeability increases, these constrictions become less restrictive and flow paths within the 2D plane become more continuous. The results show that under these conditions the extra 3D bypass routes [46] matter less, and the relative 2D–3D difference decreases with permeability (Fig. 3e).

The Overlapping Spheres medium shows earlier breakthrough in the 2D simulations than in the 3D simulations at low permeability (Fig. 3c). This can be explained, in part, by pores that are already large and interconnected in multiple directions, even at low porosity and permeability, and by the fact that some 2D slices happen to have a porosity noticeably above the 3D domain (e.g., $\phi_{2D} \approx 0.53\text{--}0.61$ at $\phi_{3D} = 0.4$), yielding higher permeabilities. At higher porosity and higher permeability, the 3D simulations appear to make greater use of additional out-of-plane flow routes that let solutes move around the spheres, routes that do not exist in the 2D slices. For M_1 , individual 2D slices with similar permeabilities both substantially under- and overpredict the 3D breakthrough (Fig. 3c), so the 2D–3D differences show no clear trend with permeability (regression slope 0.18 ± 0.07 , $R^2 = 0.28$). For the coefficient of variation, the regression slope is

small and not statistically distinguishable from zero, so the 2D–3D differences show no clear trend with permeability and go in both directions [47].

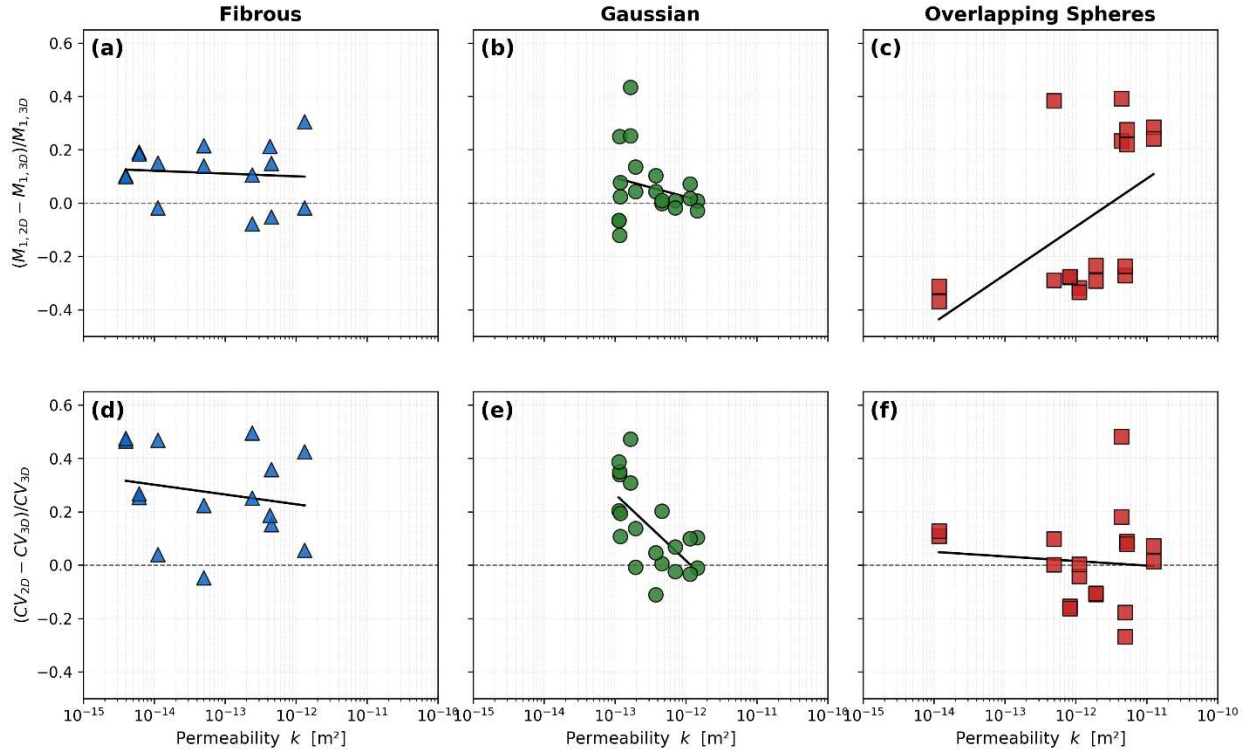


Fig. 3 Dimensional response of the conservative (unreactive) tracer across three porous media types: Fibrous (a, d), Gaussian (b, e), and Overlapping Spheres (c, f). Top row (a–c): first moment (M_1); bottom row (d–f): coefficient of variation (CV). Each panel plots the relative difference between 2D and 3D simulations, computed as $(\text{value}_{2D} - \text{value}_{3D})/\text{value}_{3D}$, against the permeability of the 2D simulation. All six panels share the same y-axis range. The solid black line in each panel is a linear regression of the relative difference on $\log_{10}k$ for that medium. Detailed regression statistics (slope, standard error, R^2 , p-value) are listed in Table C1 of Online Resource 3

3.3.2 Impact of reactivity

To assess how the reactivity of a tracer influences the difference between 2D and 3D simulations, we compare unreactive tracer simulations with a tracer that is produced at a constant rate, capturing fluid age. If pore structure controls the dimensional bias, then both tracers should behave similarly regardless of their differences in reactivity. To evaluate this, we compared the relative 2D–3D differences in breakthrough timing (M_1) and spreading (CV) for both tracers across all media (Fig. 4). The first Damköhler number in our reactive tracer simulations is well above one in all simulations, so the reaction rate is significant in our setting.

Even so, the 2D vs 3D differences in tracer arrival are governed by pore-scale flow and geometry rather than by the reaction rate itself.

Direct comparison of these metrics between reactive and unreactive tracer simulations shows that most points lie close to the 1:1 line (Fig. 4), with R^2 values between 0.94 and 0.99 for mean travel time (M_1 , top row) and between 0.34 and 0.79 for breakthrough spreading (CV, bottom row). For the mean travel time, all three media exhibit 100% (Fibrous and Gaussian) or 94% (Overlapping Spheres) of points within the $\pm 20\%$ similarity band which indicates similar outcomes between tracer types. Breakthrough spreading shows more variability: For the Fibrous, Gaussian and Overlapping Spheres media, 53, 75 and 89% of the relative CV differences are within the $\pm 20\%$ similarity band, respectively, which highlights the tracer-dependent differences. Table C2 (Online Resource 3) presents the second test: whether the best-fit slope through all pairs is equal to 1. A slope not equal to 1 indicates a systematic proportional bias between the two tracer types, independent of how close each pair lies to the 1:1 line. For M_1 the slopes are 0.72–0.81 in all three media ($p < 0.001$), so on average the reactive tracer's 2D–3D difference is 20–40% larger than the conservative one's. For CV the slope is not equal to 1 only in the Gaussian medium (2.83, $p < 0.001$), where the conservative tracer's 2D–3D difference is about 2.8× larger than the reactive one's. Fibrous and Overlapping Spheres show no such bias (slopes 1.52 and 1.74, both $p > 0.2$).

The relative 2D–3D differences in M_1 for all three media lie close to and slightly below the 1:1 line (Fig. 4, top row; slopes 0.72–0.81, Table C2, Online Resource 3), which indicates that the reactive tracer's 2D–3D difference is systematically 20–40% larger than the conservative tracer's.

In contrast, the relative difference in breakthrough spreading (Fig. 4, bottom row) are above the 1:1 line, which means that the reactive tracer overestimates the 2D–3D spreading difference relative to the conservative tracer. The magnitude of this effect depends on pore structure: In the Fibrous medium, most points are far above the 1:1 line, showing that the reactive tracer predicts much larger 2D–3D difference in CV values than the conservative tracer. In the Gaussian medium, the points still exceed the 1:1 line, but less so, showing a moderate difference between the tracers. In the Overlapping Spheres medium, many points lie close to the 1:1 line, indicating that the reactive and conservative tracers give similar 2D–3D differences in CV values.

Across the $Pe = 4.1$ –37.5 and $Da_1 > 1$ range tested here, pore structure controls the magnitude of the 2D–3D differences. For each individual simulation, the reactive and conservative tracers give similar relative 2D–3D differences in both M_1 and CV, with most pairs falling within the $\pm 20\%$ band around the 1:1 line (Fig. 4). Although each individual pair is close to the 1:1 line, the regression slope differs from 1. For M_1 , the reactive tracer's 2D–3D difference is 20–40% larger

than the conservative tracer's in all three media (slopes 0.72–0.81, Table C2, Online Resource 3), indicating that the relative 2D–3D difference in breakthrough becomes larger at larger discrepancies for the reactive than the unreactive tracer. For CV, the regression slope exceeds 1, revealing the opposite pattern for the extent of spreading. This bias appears only in the Gaussian medium, where the conservative tracer's 2D–3D difference is about 2.8× larger than the reactive one's (slope 2.83). Notably, all three CV slopes are greater than 1 (Fibrous 1.52, Gaussian 2.83, Overlapping Spheres 1.74), indicating that the direction of the bias is consistent across media, with the conservative tracer's 2D–3D difference tending to exceed the reactive one's; the Fibrous and Overlapping Spheres slopes are not distinguishable from 1 within uncertainty (both $p > 0.2$), and only the Gaussian case reaches statistical significance.

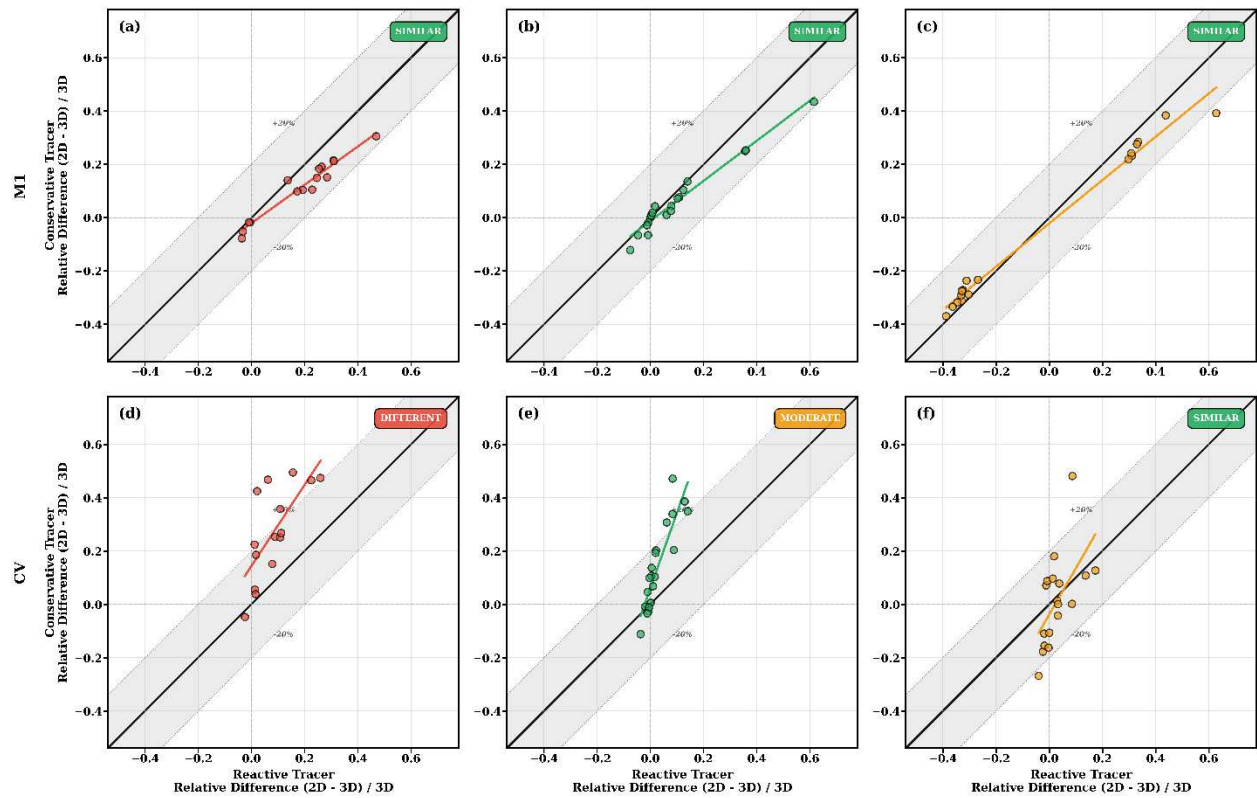


Fig. 4 Comparison of the response to dimensional reduction of reactive (x-axis) vs conservative (y-axis) tracers across Fibrous (a, d), Gaussian (b, e), and Overlapping Spheres (c, f) porous media. Top row (a–c): first moment (M_1); bottom row (d–f): coefficient of variation (CV). Each point represents a paired simulation case (same slice, porosity, and Péclet number). The black diagonal 1:1 line represents perfect agreement between tracer types, with the gray band indicating differences $< \pm 20\%$. Classification labels indicate similarity: SIMILAR ($\geq 80\%$ of points within band), MODERATE (60–79%), or DIFFERENT ($< 60\%$). Colored lines show fitted regression lines for each medium. Regression slopes different from 1 indicate systematic differences between tracer responses. Statistical tests for whether each slope significantly

differs from 1 (H_0 : slope = 1), including slope values, standard errors, 95% confidence intervals, and p-values, are provided in Table C2 of Online Resource 3

4. Conclusion

We asked whether and under what conditions two-dimensional pore scale models can meaningfully stand in for three-dimensional systems when estimating permeability, breakthrough behavior, and residence times. Our results suggest that even after Kozeny–Carman porosity correction, permeability of 2D slices systematically falls below the permeability of the 3D domain as dimensional reduction removes out of plane connections and increases tortuosity.

The 2D–3D gap in mean arrival time and breakthrough spreading varies with permeability yet the pattern is distinct between porous medium: in Fibrous domains, the offset remains nearly constant across the permeability range; in Gaussian structures, the gap decreases as permeability increases; in Overlapping Spheres, the 2D vs 3D differences are larger and go in both directions, with no clear trend with permeability. Reactive and conservative tracers show similar dimensional responses, with comparable mean travel time across all media and diverging in only one of six scenarios tested which demonstrates that pore geometry and connectivity (not tracer type) primarily govern dimensional bias.

The pore-normalized Euler characteristic $\tilde{\chi}$ offers a direct topological screening for the 2D–3D permeability gap. The largest 2D–3D differences in our simulations occur when 2D and 3D $\tilde{\chi}$ differ in sign or in magnitude (large symmetric percentage difference). Because $\tilde{\chi}$ is computed from the binary geometry alone and requires no transport simulation, it can be used before running any flow calculation: from a stack of candidate 2D slices, pick the one whose $\tilde{\chi}$ agrees in sign with the 3D parent and gives the smallest symmetric percentage difference, and use that slice as a stand-in; otherwise run the 3D simulation directly (see Fig. A14 in Online Resource 1 for the full decision pipeline). As a consequence, when constructing 2D micromodels to represent 3D systems, such as microfluidic devices, we propose that not only should one match porosity, (reactive) surface areas, but also this measure of pore scale connectivity.

References

1. Aruna, A., Barik, S., Karmakar, T., Raja Sekhar, G.P.: Multi-scale analysis of solute transport in hydrodynamic fluid flows through a porous channel with anisotropic permeability and boundary absorption. *J Eng Math.* (2024). <https://doi.org/10.1007/s10665-024-10410-x>
2. Saeibehrouzi, A., Denissenko, P., Holtzman, R., Kantsler, V., Abolfathi, S.: Solute spreading enhancement by drainage-imbibition cycles in unsaturated porous media. *Water Research.* (2025). <https://doi.org/10.1016/j.watres.2025.123741>

3. Wang, Q., Li, C., Li, Y., Zhu, R., Zhang, D.: Pore-scale study of mineral reactions in the near-wellbore region for CO₂ storage in deep saline aquifers. *Physics of Fluids*, (2025). <https://doi.org/10.1063/5.0245295>
4. Blunt, M.J., Bijeljic, B., Dong, H., Gharbi, O., Iglauer, S., Mostaghimi, P., Paluszny, A., Pentland, C.: Pore-scale imaging and modelling. *Advances in Water resources*, (2013). <https://doi.org/10.1016/j.advwatres.2012.03.003>
5. Bijeljic, B., Raeini, A., Mostaghimi, P., Blunt, M.J.: Predictions of non-Fickian solute transport in different classes of porous media using direct simulation on pore-scale images. *Phys. Rev. E*. 87, 013011 (2013). <https://doi.org/10.1103/PhysRevE.87.013011>
6. Dentz, M., Le Borgne, T., Englert, A., Bijeljic, B.: Mixing, spreading and reaction in heterogeneous media: A brief review. *Journal of Contaminant Hydrology*. 120–121, 1–17 (2011). <https://doi.org/10.1016/j.jconhyd.2010.05.002>
7. Bijeljic, B., Mostaghimi, P., Blunt, M.J.: Signature of Non-Fickian Solute Transport in Complex Heterogeneous Porous Media. *Phys. Rev. Lett.* 107, 204502 (2011). <https://doi.org/10.1103/PhysRevLett.107.204502>
8. Hajizadeh, A., Farhadpour, Z.: An Algorithm for 3D Pore Space Reconstruction from a 2D Image Using Sequential Simulation and Gradual Deformation with the Probability Perturbation Sampler. *Transp Porous Med.* 94, 859–881 (2012). <https://doi.org/10.1007/s11242-012-0028-7>
9. Fager, C., Gebäck, T., Hjärtstam, J., Röding, M., Olsson, A., Lorén, N., von Corswant, C., Särkkä, A., Olsson, E.: Correlating 3D porous structure in polymer films with mass transport properties using FIB-SEM tomography. *Chemical Engineering Science: X*. 12, 100109 (2021). <https://doi.org/10.1016/j.cesx.2021.100109>
10. Lee, W., Chen, M.A., Bresciani, E., Toner, B.M., Kang, P.K.: Effects of Pore-Scale Three-Dimensional Flow and Fluid Inertia on Mineral Dissolution. *Water Resources Research*. 61, e2024WR038176 (2025). <https://doi.org/10.1029/2024WR038176>
11. Marafini, E., La Rocca, M., Fiori, A., Battiato, I., Prestininzi, P.: Suitability of 2D modelling to evaluate flow properties in 3D porous media. *Transport in Porous Media*, (2020). <https://doi.org/10.1007/s11242-020-01447-4>
12. Lemaitre, R., Adler, P.: Fractal porous media IV: three-dimensional stokes flow through random media and regular fractals. *Transport in Porous Media*, (1990). <https://doi.org/10.1007/BF01141990>
13. Adler, P.M., Jacquin, C.G., Thovert, J.: The formation factor of reconstructed porous media. *Water resources research*. 28, (1992). <https://doi.org/10.1029/92WR00059>
14. Knudsen, H.A., Aker, E., Hansen, A.: Bulk flow regimes and fractional flow in 2D porous media by numerical simulations. *Transport in Porous Media*, (2002). <https://doi.org/10.1023/A:1015039503551>
15. Duda, A., Koza, Z., Matyka, M.: Hydraulic tortuosity in arbitrary porous media flow. *Physical Review E—Statistical, Nonlinear, and Soft Matter Physics*. 84, 036319 (2011). <https://doi.org/10.1103/PhysRevE.84.036319>
16. Koponen, A., Kataja, M., Timonen, J.: Permeability and effective porosity of porous media. *Physical Review E*, (1997). <https://doi.org/10.1103/PhysRevE.56.3319>

17. Naraghi, M.E., Spikes, K., Srinivasan, S.: 3D Reconstruction of Porous Media From a 2D Section and Comparisons of Transport and Elastic Properties. *Spe Reservoir Evaluation & Engineering*. 20, 342–352 (2017). <https://doi.org/10.2118/180489-PA>
18. Herring, A.L., Robins, V., Sheppard, A.P.: Topological persistence for relating microstructure and capillary fluid trapping in sandstones. *Water Resources Research*, (2019). <https://doi.org/10.1029/2018WR022780>
19. Robins, V., Saadatfar, M., Delgado-Friedrichs, O., Sheppard, A.P.: Percolating length scales from topological persistence analysis of micro- CT images of porous materials. *Water Resources Research*. 52, 315–329 (2016). <https://doi.org/10.1002/2015WR017937>
20. Khanafer, K., AlAmiri, A., Pop, I., Bull, J.L.: Flow and Heat Transfer in Biological Tissues: Application of Porous Media Theory. In: Vadász, P. (ed.) *Emerging Topics in Heat and Mass Transfer in Porous Media: From Bioengineering and Microelectronics to Nanotechnology*. pp. 237–259. Springer Netherlands, Dordrecht (2008)
21. Kuts, M., Walker, J., Newell, P.: Computational homogenization of linear elastic properties in porous non-woven fibrous materials. *Mechanics of Materials*. 189, 104868 (2024). <https://doi.org/10.1016/j.mechmat.2023.104868>
22. Abdi, R., Krzaczek, M., Tejchman, J.: Simulations of high-pressure fluid flow in a pre-cracked rock specimen composed of densely packed bonded spheres using a 3D CFD model and simplified 2D coupled CFD-DEM approach. *Powder Technology*. 417, 118238 (2023). <https://doi.org/10.1016/j.powtec.2023.118238>
23. Latief, F.D.E., Pantouw, G.T., Wongkaren, H.J., Amien, N.: Implementation of overlap degree in sphere packed sedimentary rock model and its impact to pore structure characteristics. *IOP Conf. Ser.: Earth Environ. Sci.* 311, 012042 (2019). <https://doi.org/10.1088/1755-1315/311/1/012042>
24. Latief, F.D.E., Fauzi, U.: Pore shape characterization of Fontainebleau sandstone and its models using Fourier descriptor. *AIP Conference Proceedings*. 1589, 72–75 (2014). <https://doi.org/10.1063/1.4868753>
25. Zhao, L., Li, H., Meng, J., Zhang, D.: Efficient uncertainty quantification for permeability of three-dimensional porous media through image analysis and pore-scale simulations. *Phys. Rev. E*. 102, 023308 (2020). <https://doi.org/10.1103/PhysRevE.102.023308>
26. Du, R., Liu, Z.: A lattice Boltzmann model for the fractional advection–diffusion equation coupled with incompressible Navier–Stokes equation. *Applied Mathematics Letters*. 101, 106074 (2020). <https://doi.org/10.1016/j.aml.2019.106074>
27. Jung, H., Song, H.-S., Meile, C.: CompLaB v1.0: a scalable pore-scale model for flow, biogeochemistry, microbial metabolism, and biofilm dynamics. *Geoscientific Model Development*, (2023). <https://doi.org/10.5194/gmd-16-1683-2023>
28. Adam, S., Hajabdollahi, F., Premnath, K.N.: Cascaded lattice Boltzmann modeling and simulations of three-dimensional non-Newtonian fluid flows. *Computer Physics Communications*, (2021). <https://doi.org/10.1016/j.cpc.2021.107858>
29. He, Y.-L., Liu, Q., Li, Q., Tao, W.-Q.: Lattice Boltzmann methods for single-phase and solid-liquid phase-change heat transfer in porous media: A review. *International Journal of Heat and Mass Transfer*. 129, 160–197 (2019). <https://doi.org/10.1016/j.ijheatmasstransfer.2018.08.135>

30. Spiller, D., Dünweg, B.: Semiautomatic construction of lattice Boltzmann models. *Phys. Rev. E.* 101, 043310 (2020). <https://doi.org/10.1103/PhysRevE.101.043310>
31. Yonekura, K., Kanno, Y.: Topology optimization method for interior flow based on transient information of the lattice Boltzmann method with a level-set function. *Japan J. Indust. Appl. Math.* 34, 611–632 (2017). <https://doi.org/10.1007/s13160-017-0257-9>
32. Asgari, S., Meile, C.: CompLaB3D: a three-dimensional pore-scale reactive transport modeling framework and graphical user interface coupling lattice Boltzmann flow with biogeochemical kinetics, equilibrium chemistry and biofilm dynamics. *Journal of Open Source Software.* (2026)
33. Kang, Q., Lichtner, P.C., Zhang, D.: Lattice Boltzmann pore-scale model for multicomponent reactive transport in porous media. *Journal of Geophysical Research: Solid Earth.* 111, (2006). <https://doi.org/10.1029/2005JB003951>
34. Jiménez-Hornero, F.J., Giráldez, J.V., Laguna, A.: Simulation of tracer dispersion in porous media using lattice Boltzmann and random walk models. *Vadose Zone Journal*, (2005). <https://doi.org/10.2136/vzj2004.0090>
35. Goode, D.J.: Direct Simulation of Groundwater Age. *Water Resources Research.* 32, 289–296 (1996). <https://doi.org/10.1029/95WR03401>
36. Rooze, J., Jung, H., Radtke, H.: A novel Eulerian model based on central moments to simulate age and reactivity continua interacting with mixing processes. *Geoscientific Model Development*, (2023). <https://doi.org/10.5194/gmd-16-7107-2023>
37. Wagner, H., Chen, C., Vućini, E.: Efficient computation of persistent homology for cubical data. In: *Topological methods in data analysis and visualization II*, Springer (2011). https://doi.org/10.1007/978-3-642-23175-9_7
38. Ávila, J., Pagalo, J., Espinoza-Andaluz, M.: Evaluation of geometric tortuosity for 3D digitally generated porous media considering the pore size distribution and the A-star algorithm. *Scientific reports*, (2022). <https://doi.org/10.1038/s41598-022-23643-6>
39. Bernabé, Y., Li, M., Maineult, A.: Permeability and pore connectivity: a new model based on network simulations. *Journal of Geophysical Research: Solid Earth.* 115, (2010). <https://doi.org/10.1029/2010JB007444>
40. Beckingham, L.E., Peters, C.A., Um, W., Jones, K.W., Lindquist, W.B.: 2D and 3D imaging resolution trade-offs in quantifying pore throats for prediction of permeability. *Advances in water resources*, (2013). <https://doi.org/10.1016/j.advwatres.2013.08.010>
41. Payton, R.L., Chiarella, D., Kingdon, A.: The upper percolation threshold and porosity–permeability relationship in sandstone reservoirs using digital image analysis. *Scientific Reports*, (2022). <https://doi.org/10.1038/s41598-022-15651-3>
42. Huang, X., Zhao, J., Zhou, Z., Yang, D., Wang, G., Kang, Z.: 3D Percolation Modeling for Connectivity and Permeability of Sandstone with Different Pore Distribution Characteristics. *Natural Resources Research*, (2024). <https://doi.org/10.1007/s11053-023-10277-2>
43. Vallabh, R., Banks-Lee, P., Seyam, A.-F.: New approach for determining tortuosity in fibrous porous media. *Journal of Engineered Fibers and Fabrics*, (2010). <https://doi.org/10.1177/155892501000500302>

44. Renard, P., Allard, D.: Connectivity metrics for subsurface flow and transport. *Advances in Water Resources*, (2013). <https://doi.org/10.1016/j.advwatres.2011.12.001>
45. Lester, D.R., Dentz, M., Le Borgne, T.: Chaotic mixing in three-dimensional porous media. *Journal of Fluid Mechanics*, (2016). <https://doi.org/10.1017/jfm.2016.486>
46. Yang, X., Mehmani, Y., Perkins, W.A., Pasquali, A., Schönherr, M., Kim, K., Perego, M., Parks, M.L., Trask, N., Balhoff, M.T.: Intercomparison of 3D pore-scale flow and solute transport simulation methods. *Advances in water resources*, (2016). <https://doi.org/10.1016/j.advwatres.2015.09.015>
47. Aramideh, S., Vlachos, P.P., Ardekani, A.M.: Pore-scale statistics of flow and transport through porous media. *Physical Review E*. (2018). <https://doi.org/10.1103/PhysRevE.98.013104>

Statements and Declarations

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Data Availability The datasets generated and analyzed during the current study are available from the corresponding author on reasonable request.

Code Availability The ComLaB3D code used in this study [32] is available on Zenodo at <https://doi.org/10.5281/zenodo.19964835> and on GitHub at <https://github.com/shahram444/Complab3D-Biotic-Kinetic-AndersopnNR>.

Declaration of generative AI and AI-assisted technologies in the manuscript preparation process During the preparation of this work the authors used Claude (Anthropic) in order to improve the language and readability of text that the authors had written. After using this tool, the authors reviewed and edited the content as needed and take full responsibility for the content of the published article.

Supplementary Information

Online Resource 1 Persistent-homology connectivity analysis of the pore networks.

Online Resource 2 Domain-size and microstructure analysis.

Online Resource 3 Breakthrough curves, temporal moments and regression statistics.

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