

Online Resource 3

Breakthrough curves, temporal moments and regression statistics

C1. Breakthrough curves and temporal moments

To investigate the role of pore geometry and dimensionality on solute migration, we computed flux-weighted breakthrough curves (BTCs) for all porous media types under systematically varied porosity and Péclet number conditions (Fig. C1). For each case, the 3D breakthrough response was compared against representative 2D BTCs using temporal moments.

The n-th raw temporal moment of the breakthrough concentration is defined as (Kreft and Zuber 1978):

$$M_n = \frac{\int_0^\infty t^n C(t) dt}{\int_0^\infty C(t) dt}$$

where $C(t)$ is the flux-weighted concentration at the outlet and t is time. The mean travel time is hence captured by the first moment (M_1) and the variability (σ) around the mean is captured by the square root of the second central moment (Cirpka and Kitanidis 2000; Guleria et al. 2020):

$$\sigma = \sqrt{\frac{\int_0^\infty (t-M_1)^2 C(t) dt}{\int_0^\infty C(t) dt}} = \sqrt{M_2 - M_1^2}$$

To compare solute spreading across systems with different flow velocities, we used the coefficient of variation (CV), a dimensionless measure of relative spreading:

$$CV = \frac{\sigma}{M_1}$$

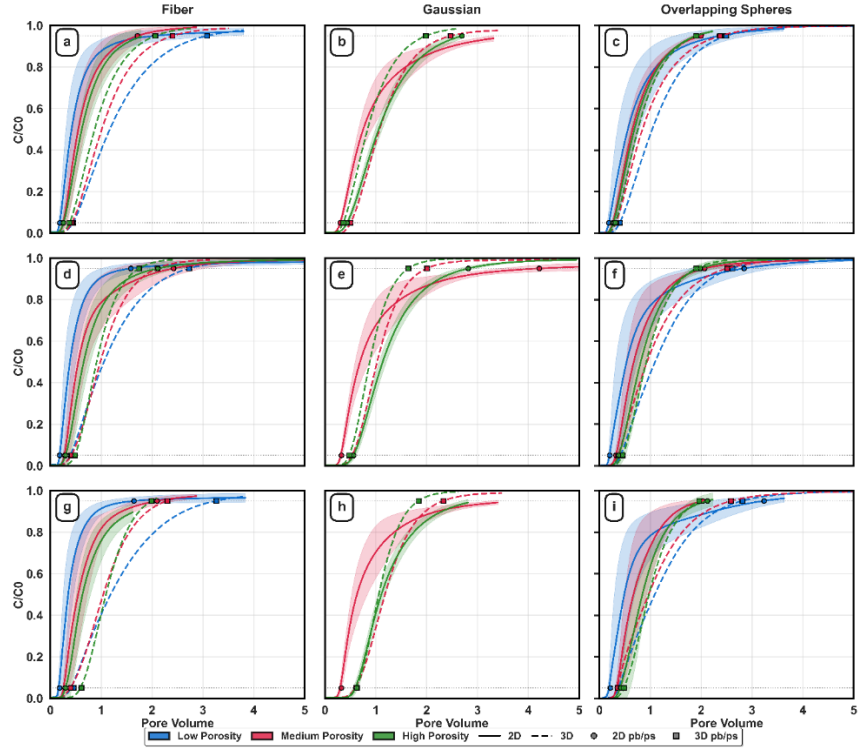


Fig. C1 Flux-weighted breakthrough curves (normalized outlet concentration C/C_0 versus pore volumes injected) for the Fibrous (a, d, g), Gaussian (b, e, h) and Overlapping Spheres (c, f, i) media at low (blue), medium (red) and high (green) porosity, comparing 2D slices (solid lines; shaded bands span the slice-to-slice range) with the corresponding 3D domains (dashed lines) at the three Péclet numbers investigated (rows). Circles and squares mark the 2D and 3D breakthrough points, respectively

C2. Statistical analysis tables

To quantify to what extent 2D and 3D results differ from each other across media, we fit simple linear regressions between permeability and the relative 2D–3D differences in M_1 and CV for both tracer types. The slopes and p-values in Table C1 indicate whether these dimensional differences vary significantly with permeability.

Table C1 Regression slopes ($\pm$ standard error) and p-values for the relative differences between 2D and 3D simulations for M_1 and CV across different porous media types for the conservative and reactive tracers, respectively. Bold values indicate relationships where the slope is significantly different from zero ($p < 0.05$).

Tracer Type	Metric	Medium	Slope $\pm$ SE	p-value
Conservative	$\frac{M_{1,2D} \cdot M_{1,3D}}{M_{1,3D}}$	Fibrous	-0.0104 $\pm$ 0.0323	0.7518
		Gaussian	-0.0714 $\pm$ 0.0720	0.3346

		Overlapping Spheres	0.1798 ± 0.0728	0.0252
	$\frac{CV_{2D} \cdot CV_{3D}}{CV_{3D}}$	Fibrous	-0.0366 ± 0.0503	0.4802
		Gaussian	-0.2494 ± 0.0715	0.0026
		Overlapping Spheres	-0.0171 ± 0.0492	0.7322
Reactive	$\frac{M_{1,2D} \cdot M_{1,3D}}{M_{1,3D}}$	Fibrous	-0.0072 ± 0.0438	0.8720
		Gaussian	-0.1330 ± 0.0911	0.1614
		Overlapping Spheres	$+0.2071 \pm 0.0909$	0.0369
	$\frac{CV_{2D} \cdot CV_{3D}}{CV_{3D}}$	Fibrous	-0.0394 ± 0.0214	0.0887
		Gaussian	-0.0755 ± 0.0231	0.0042
		Overlapping Spheres	-0.0480 ± 0.0115	0.0007

To test whether reactive and conservative tracers respond similarly to dimensional reduction, we compared their relative 2D–3D differences using a 1:1 slope. Here, a slope of 1 means that the two tracer types respond identically across all cases. Table C2 shows how close the slopes are to 1 and whether the differences are statistically significant. Slopes < 1 indicate reactive tracers show larger dimensional differences while slopes > 1 indicate conservative tracers show larger differences. For M_1 , all media have slopes significantly < 1 ($p < 0.001$). For CV, only Gaussian media differs significantly from 1 (slope ≈ 2.83 , $p < 0.001$), while Fibrous and Overlapping Spheres show no significant difference between reactive and unreactive tracers.

Table C2 Statistical analysis of reactive and conservative tracer behavior. For each medium and metric combination, we tested H_0 : slope = 1 (reactive and conservative tracers respond identically) vs H_1 : slope $\neq 1$ (tracers respond differently). Columns: Metric (M_1 = first moment; CV = coefficient of variation); Medium (porous medium type); Slope (regression slope of conservative vs reactive relative differences); Slope SE (standard error); p-value.

Metric	Medium	Slope	Slope SE	p-value
M_1	Fibrous	0.7194	0.048	5.6917E-05***
M_1	Gaussian	0.7526	0.0356	1.73823E-06***
M_1	Overlapping Spheres	0.8127	0.0228	3.9044E-07***
CV	Fibrous	1.522	0.4147	0.230 ^{ns}

CV	Gaussian	2.8293	0.3415	4.31437E-05***
CV	Overlapping Spheres	1.7353	0.6026	0.240 ^{ns}

*** $p < 0.001$; ns not significant ($p \geq 0.05$)

References

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