Predicting the impact of spatial heterogeneity on microbial redox dynamics and nutrient cycling in the subsurface

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Supplement

Figures

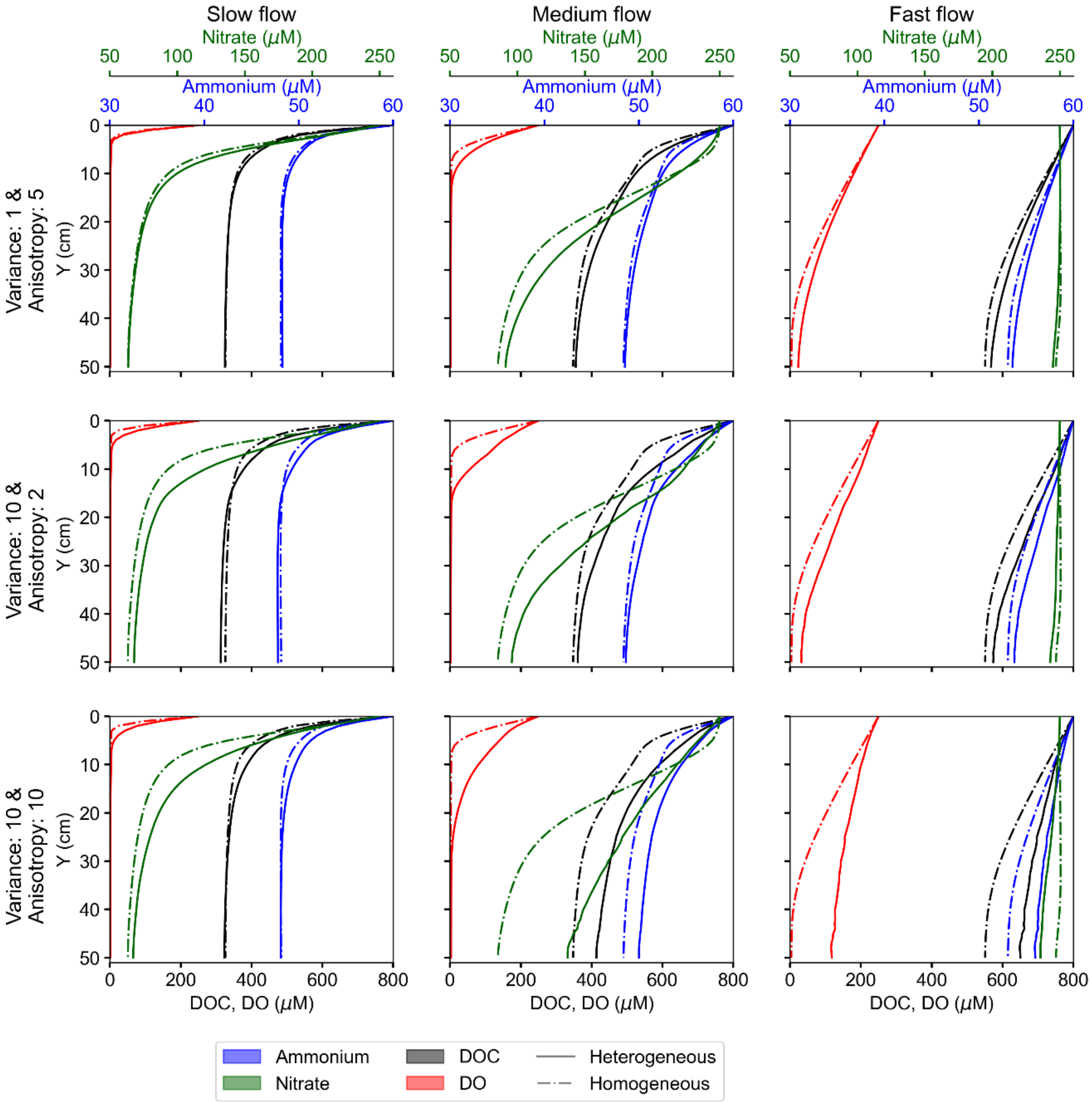

Figure S1: Flux averaged concentrations of dissolved species in heterogeneous domains in three types of heterogeneous scenarios (solid lines) compared to that in the homogeneous base case (dashed-dot lines) in all flow regimes

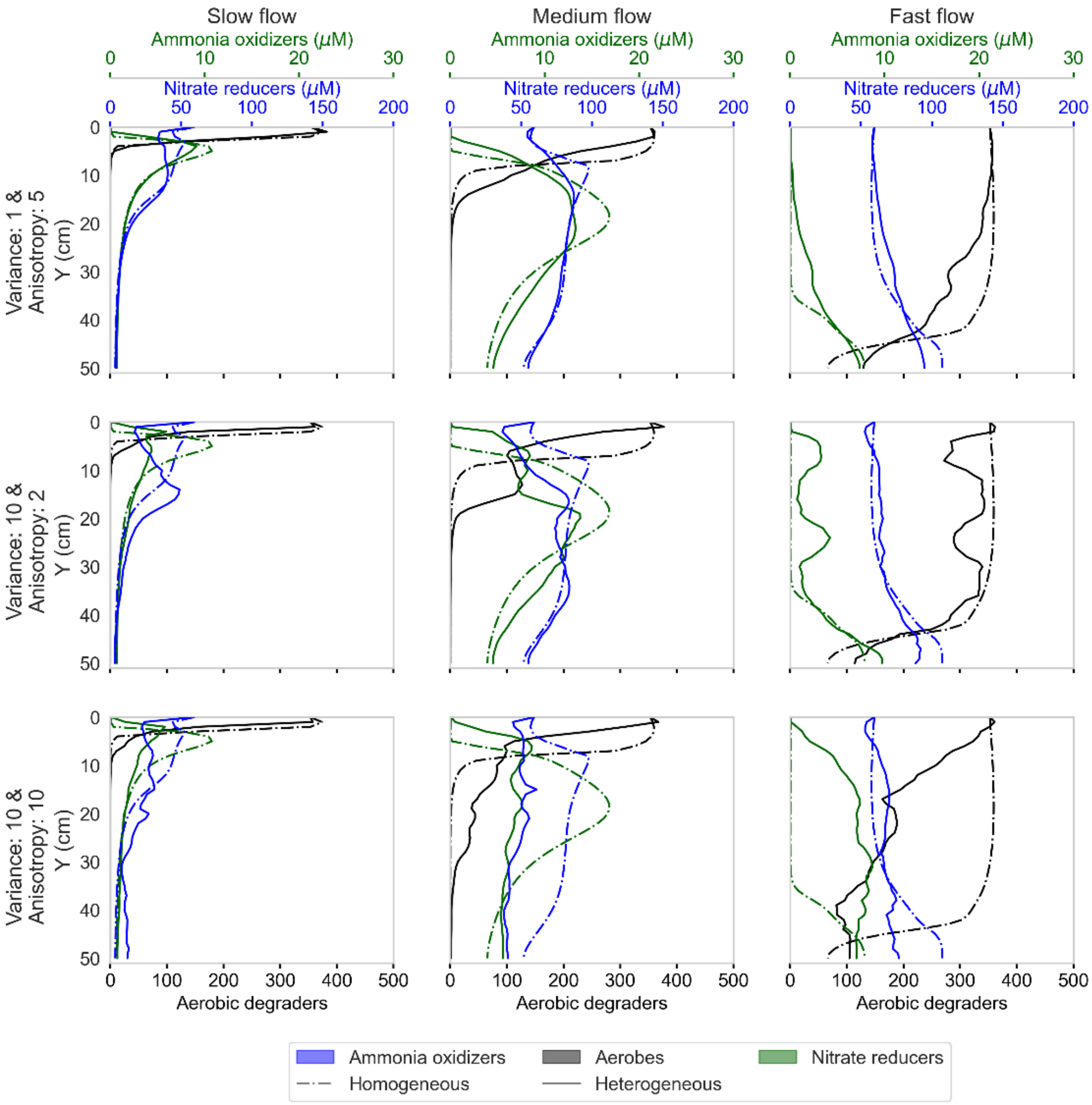

Figure S2: Spatially averaged concentration profile of the immobile active biomass in heterogeneous domains in three types of heterogeneous scenarios (solid lines) compared to that in the homogeneous base case (dashed-dot lines) in all flow regimes

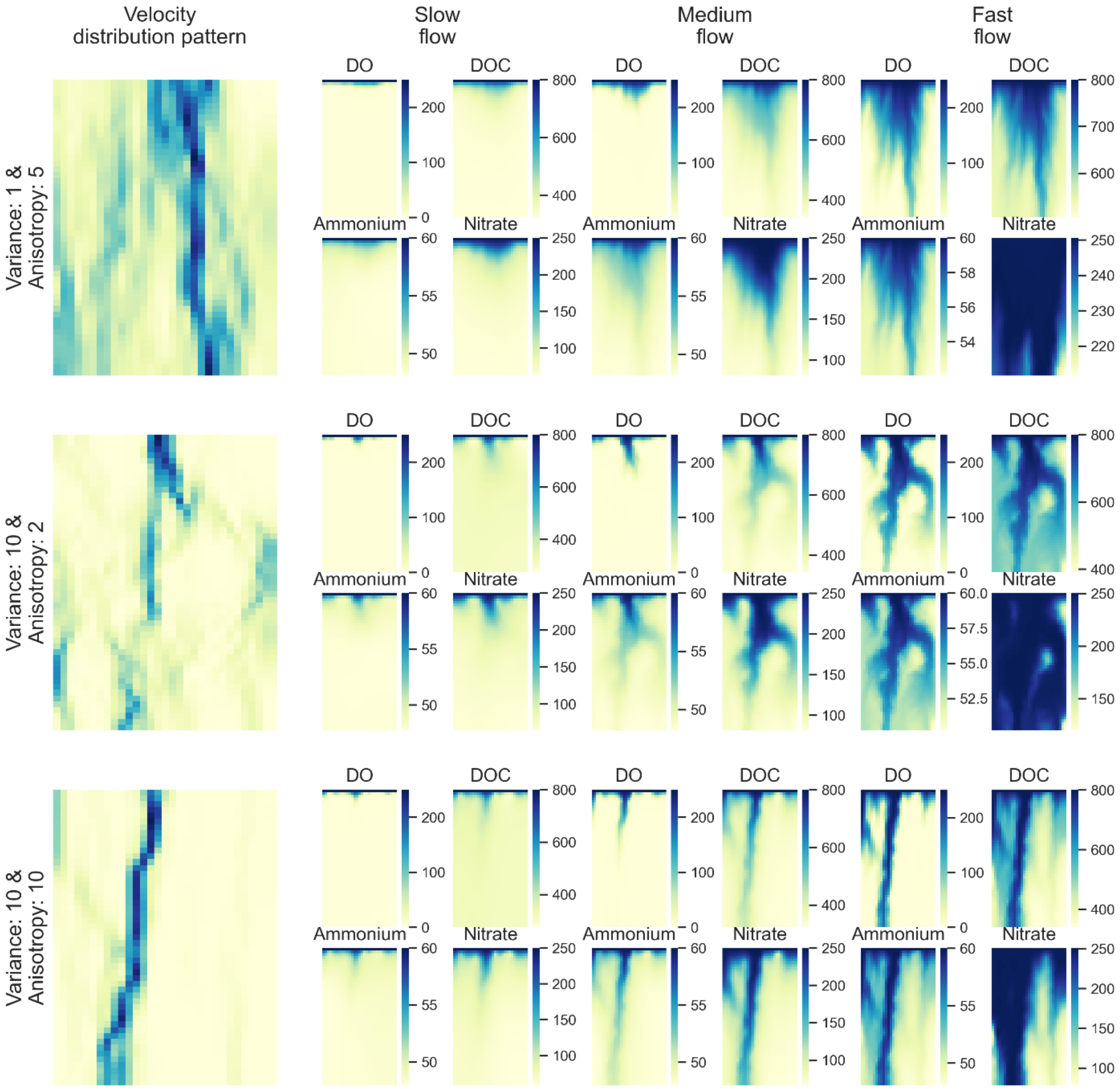

Figure S3: 2D concentration distributions of dissolved species in heterogeneous domains (µM) with the velocity distribution (in m d^{-1}) in these domains.

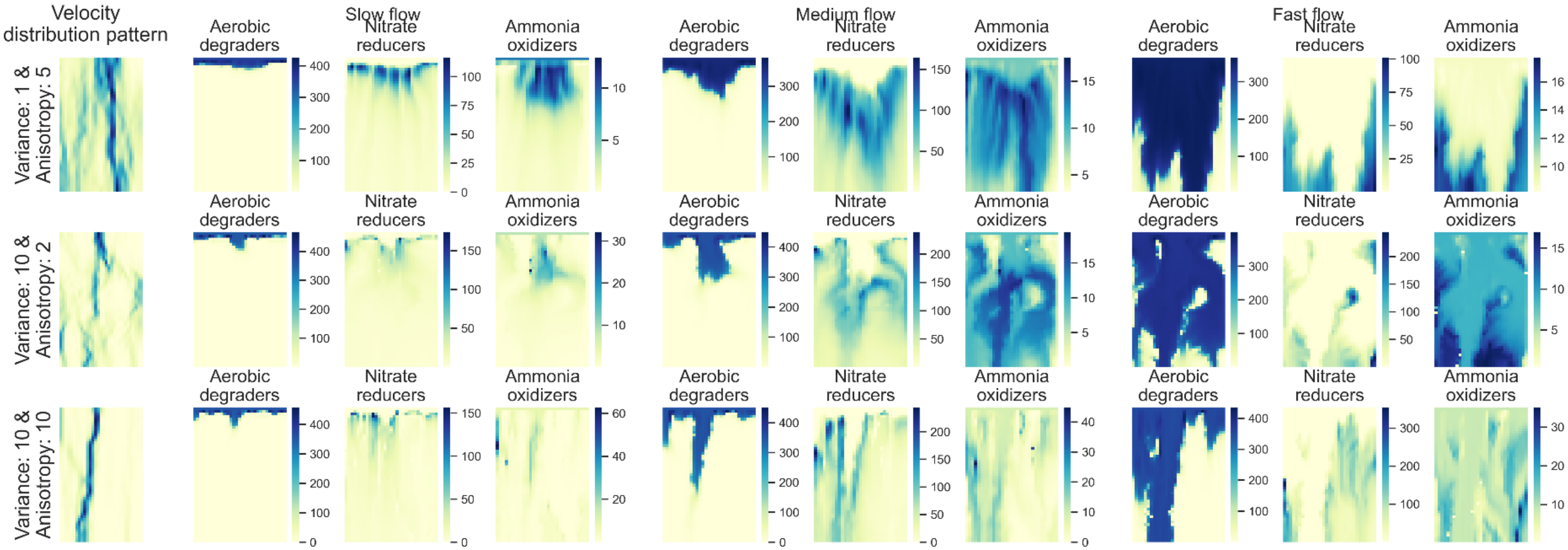

Figure S4: 2D concentration distributions of microbial species in heterogeneous domains (μM) with the velocity distribution (in m d^{-1}) in these domains

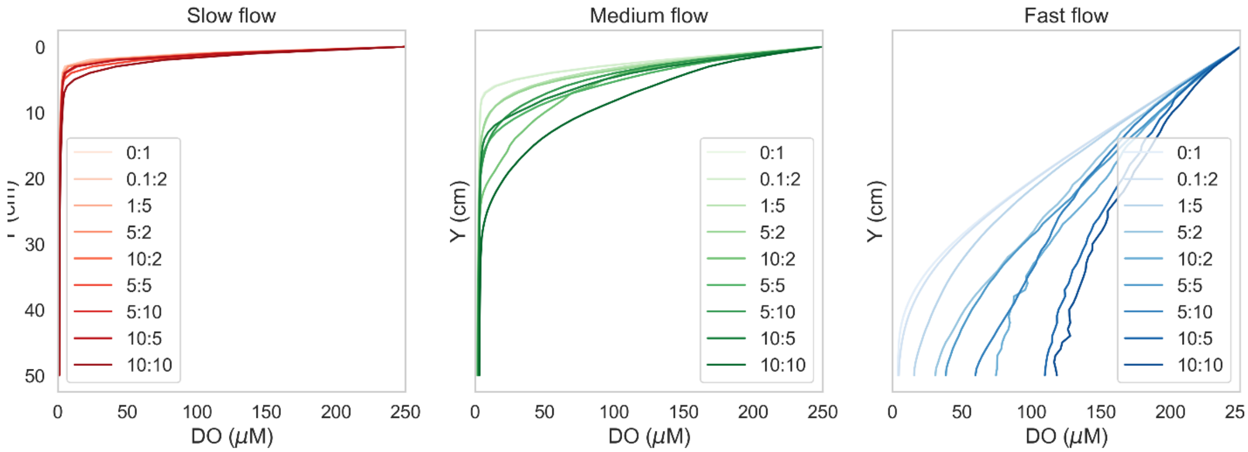

Figure S5: Increasing DO persistence with heterogeneity (presented in the legend as Variance in permeability field: Anisotropy)

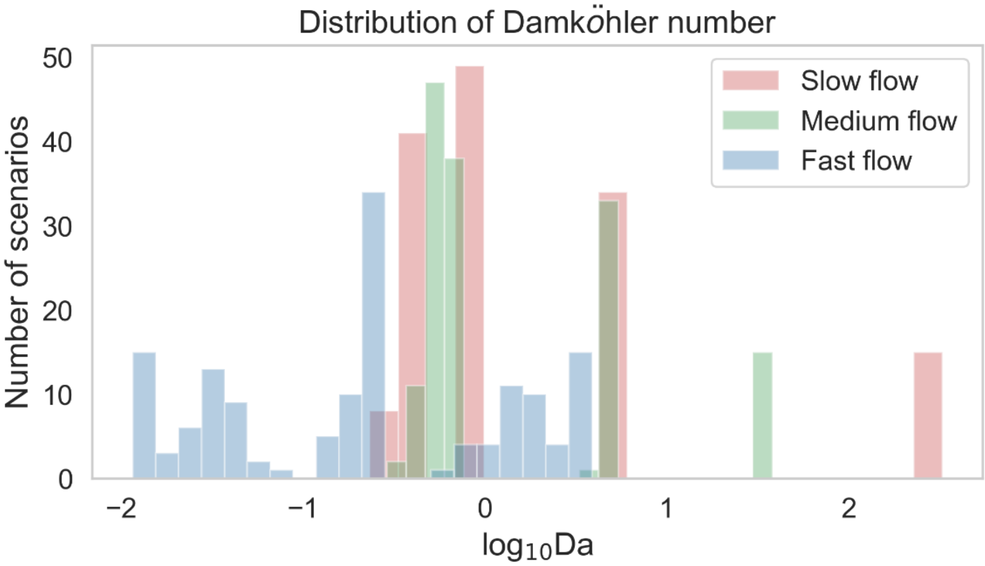

Figure S6: Distribution of Damköhler number in the investigated scenarios.

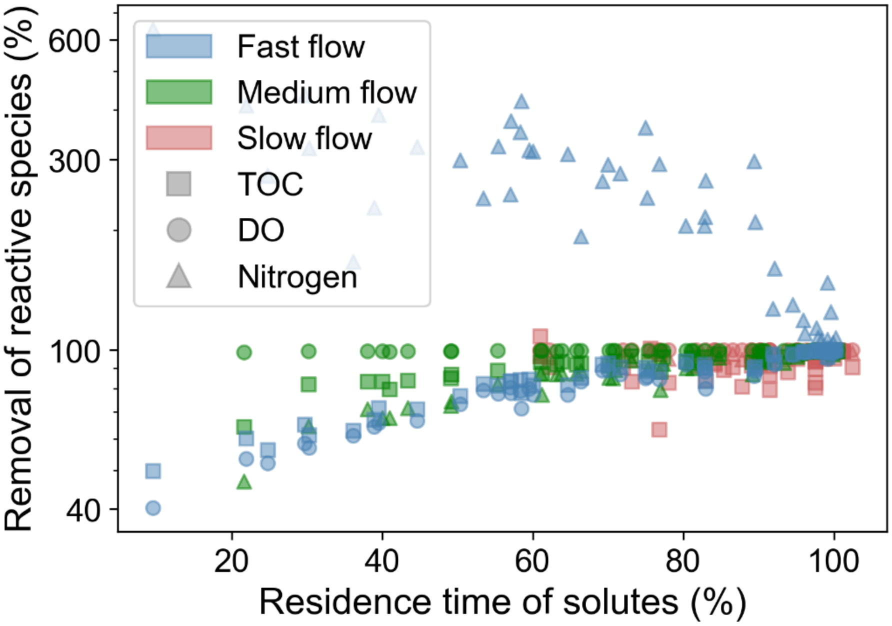

Figure S7: Impact on (normalized) removal of reactive species as a result of spatial heterogeneity characterized as reduction in solute residence times in the domain

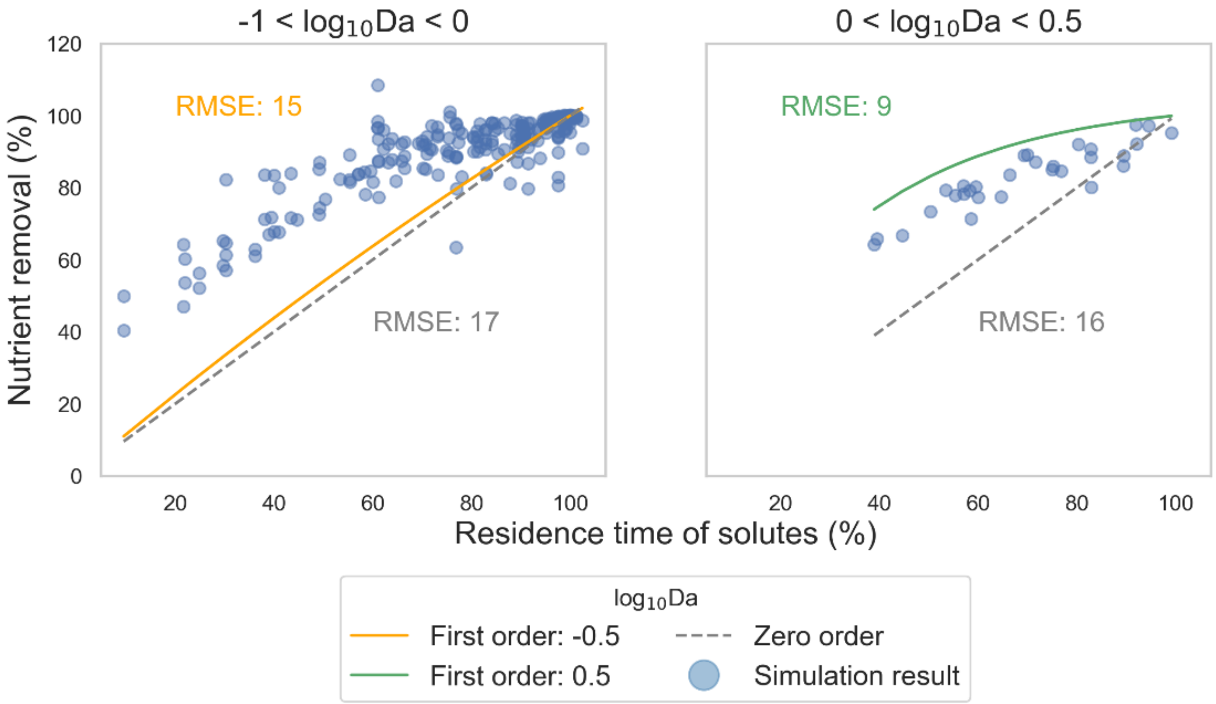

Figure S8: Comparison of simulation results and corresponding analytical solutions for changing removal of reactive species with changing residence time alone.

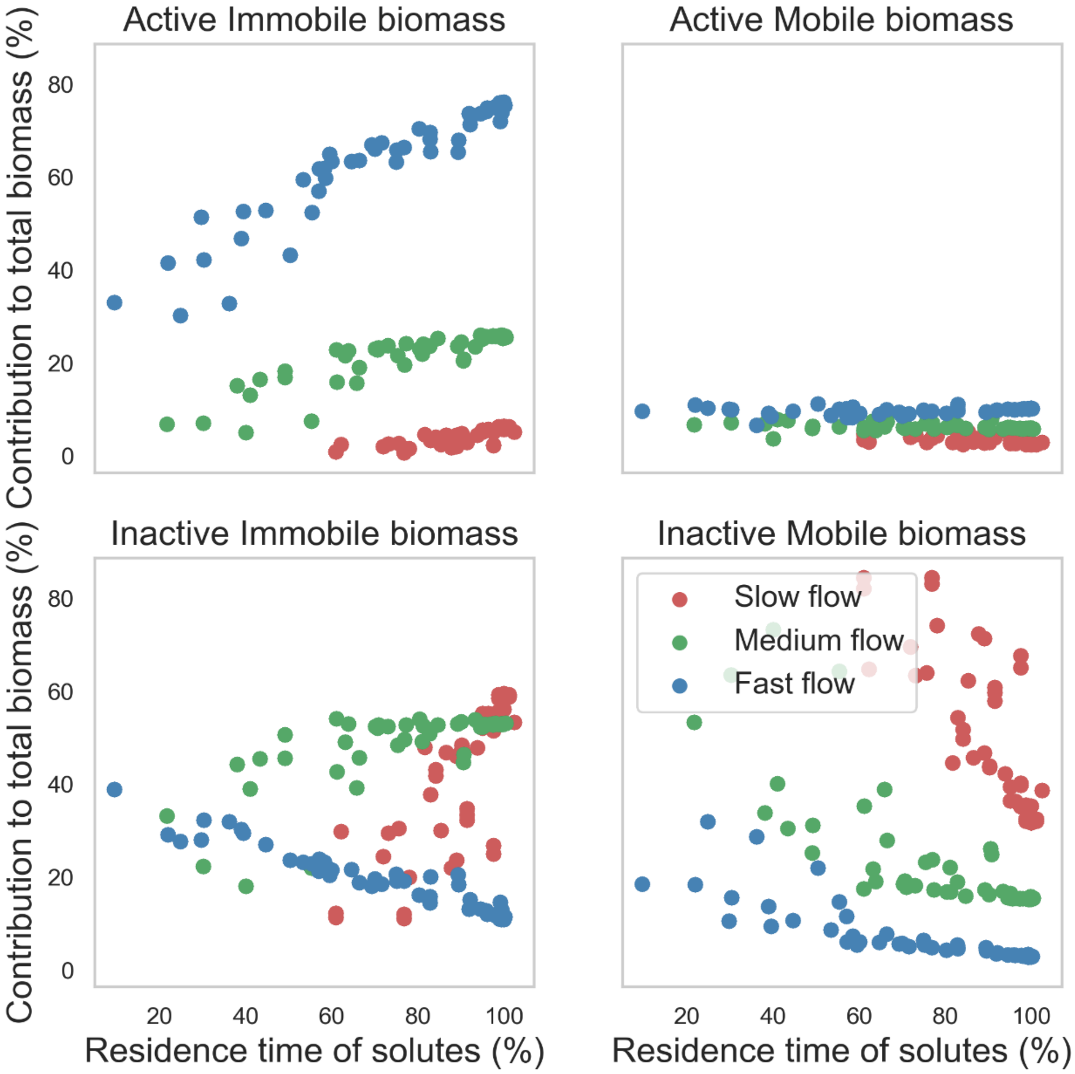

Figure S9: Contribution to total biomass of different fractions of microbial species with increasing spatial heterogeneity (i.e., decreasing residence time of solutes).

Tables

S. No.	**Independent variable/ fixed effect**	**Random effect**	**Interaction between breakthrough time and random effects**	**AIC**
1	**fraction of breakthrough time**	**Flow regime**	**No**	**904.88**
2	**fraction of breakthrough time**	**Chemical species**	**No**	**841.05**
3	**fraction of breakthrough time**	**Flow regime**	**Yes**	**896.21**
4	**fraction of breakthrough time**	**Chemical species**	**Yes**	**677.29**
5	**fraction of breakthrough time**	**Flow regime + Variance + Anisotropy + Chemical species**	**No**	**426.54**
6	**fraction of breakthrough time**	**Flow regime + Variance + Anisotropy + Chemical species**	**Yes**	**156.46**
7	**fraction of breakthrough time**	**Regime + Chemical species**	**No**	**481.84**
8	**fraction of breakthrough time**	**Regime + Chemical species**	**Yes**	**-147.75**
9	**fraction of breakthrough time + Flow regime**	**Flow regime + Variance + Anisotropy + Chemical species**	**Yes**	**148.29**
10	**fraction of breakthrough time + Flow regime**	**Regime + Chemical species**	**Yes**	**-86.47**
11	**fraction of breakthrough time + Flow regime + Chemical species**	**Regime + Chemical species**	**Yes**	**-141.27**
12	**fraction of breakthrough time + Chemical species**	**Regime + Chemical species**	**Yes**	**-142.45**
13	**fraction of breakthrough time**	**Flow regime + Variance + Anisotropy + Chemical species + Da_t category**	**Yes**	**35.87**
14	**fraction of breakthrough time**	**Flow regime + Chemical species + Da_t category**	**Yes**	**-211.06**
15	**fraction of breakthrough time + Flow regime**	**Flow regime + Variance + Anisotropy + Chemical species + Da_t category**	**Yes**	**25.39**
16	**fraction of breakthrough time + Flow regime**	**Flow regime + Chemical species + Da_t category**	**Yes**	**-209.61**
17	**fraction of breakthrough time + Flow regime + Chemical species**	**Flow regime + Variance + Anisotropy + Chemical species + Da_t category**	**Yes**	**20.18**
18	**fraction of breakthrough time + Flow regime + Chemical species**	**Flow regime + Chemical species + Da_t category**	**Yes**	**-191.36**
19	**fraction of breakthrough time + Chemical species**	**Flow regime + Variance + Anisotropy + Chemical species + Da_t category**	**Yes**	**20.72**
20	**fraction of breakthrough time + Chemical species**	**Flow regime + Chemical species + Da_t category**	**Yes**	**-180.86**

Table S1 Linear mixed models for the simulation dataset

Model:			**Dependent Variable:**		impact on species removal	
No. Observations:	588		**Method:**		REML	
No. Groups	4		**Scale:**		154.32	
Min. group size	49		**Log-Likelihood:**		-2318	
Max. group size	214		**Converged:**		Yes	
Mean group size	147					
	Coef.	**Std. Err**	**z**	**P>|z|**	**[0.025**	**0.975]**
Intercept	27.72	7.355	3.769	0	13.30	42.14
Chem [T.DOC]	-12.37	1.468	-8.429	0	-15.25	-9.497
Chem [T. Nitrogen]	-34.32	1.684	-20.38	0	-37.62	-31.02
Chem [T.TOC]	-6.741	1.449	-4.652	0	-9.581	-3.901
fraction of breakthrough time	7.086	8.989	0.788	0.431	-10.53	24.71
Group variance	187.5	14.50				
Group x fraction covariance	102.4	12.78				
fraction variance	286.3	20.26				

Table S2 Mixed linear effects model results: Summary