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Supplement of

Predicting the impact of spatial heterogeneity on microbially mediated nutrient cycling in the subsurface

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Figures

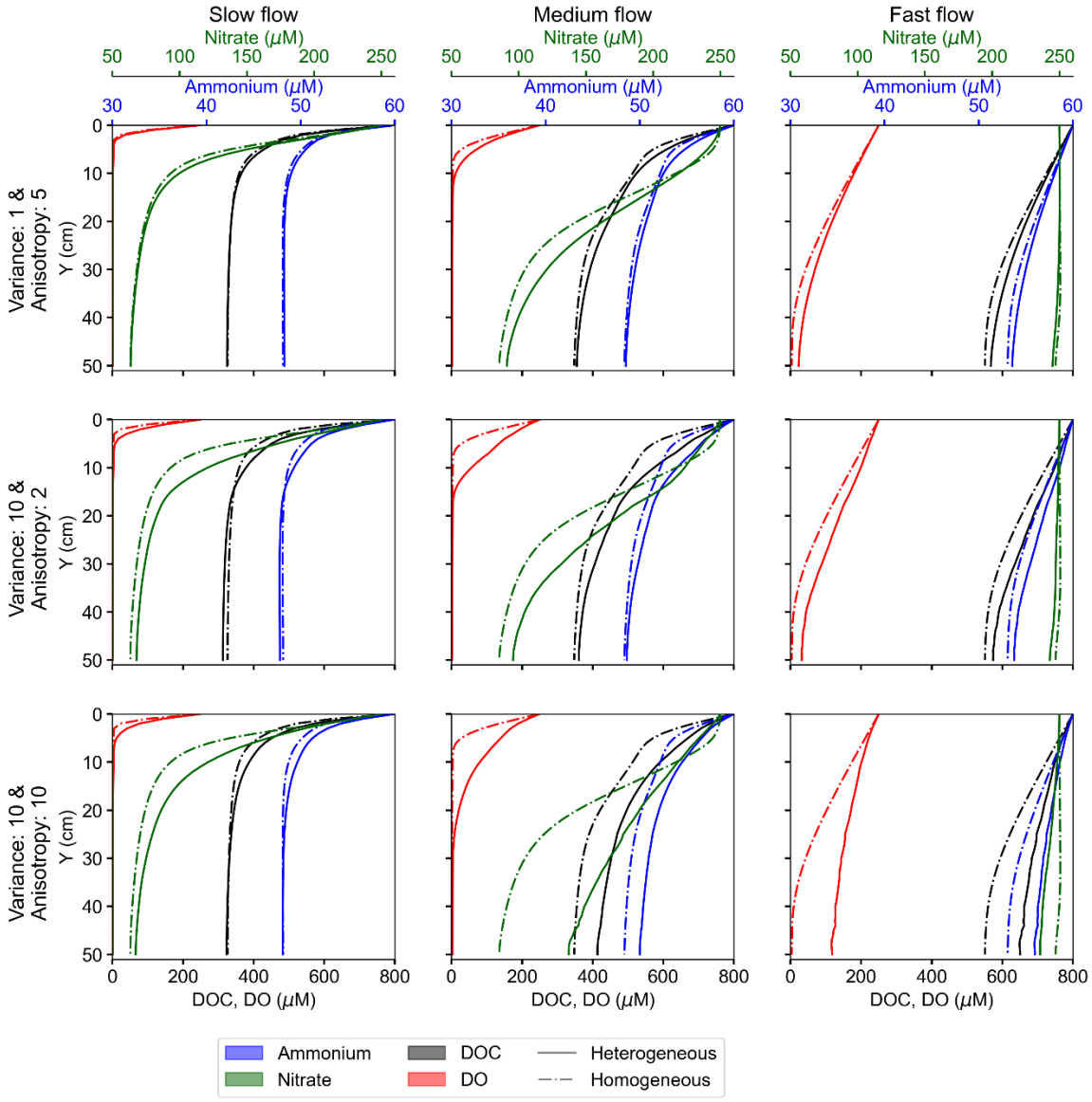


Figure S1: Flux averaged concentrations of dissolved species in heterogeneous domains (indicated by variance and anisotropy values in the row index) in three types of heterogeneous scenarios (solid lines) compared to that in the homogeneous base case (zero variance and no associated anisotropy, dashed-dot lines) in all flow regimes. The flux averaged concentration profile is the same for a given column (i.e., there is only one homogeneous/base case for comparison in each flow regime).

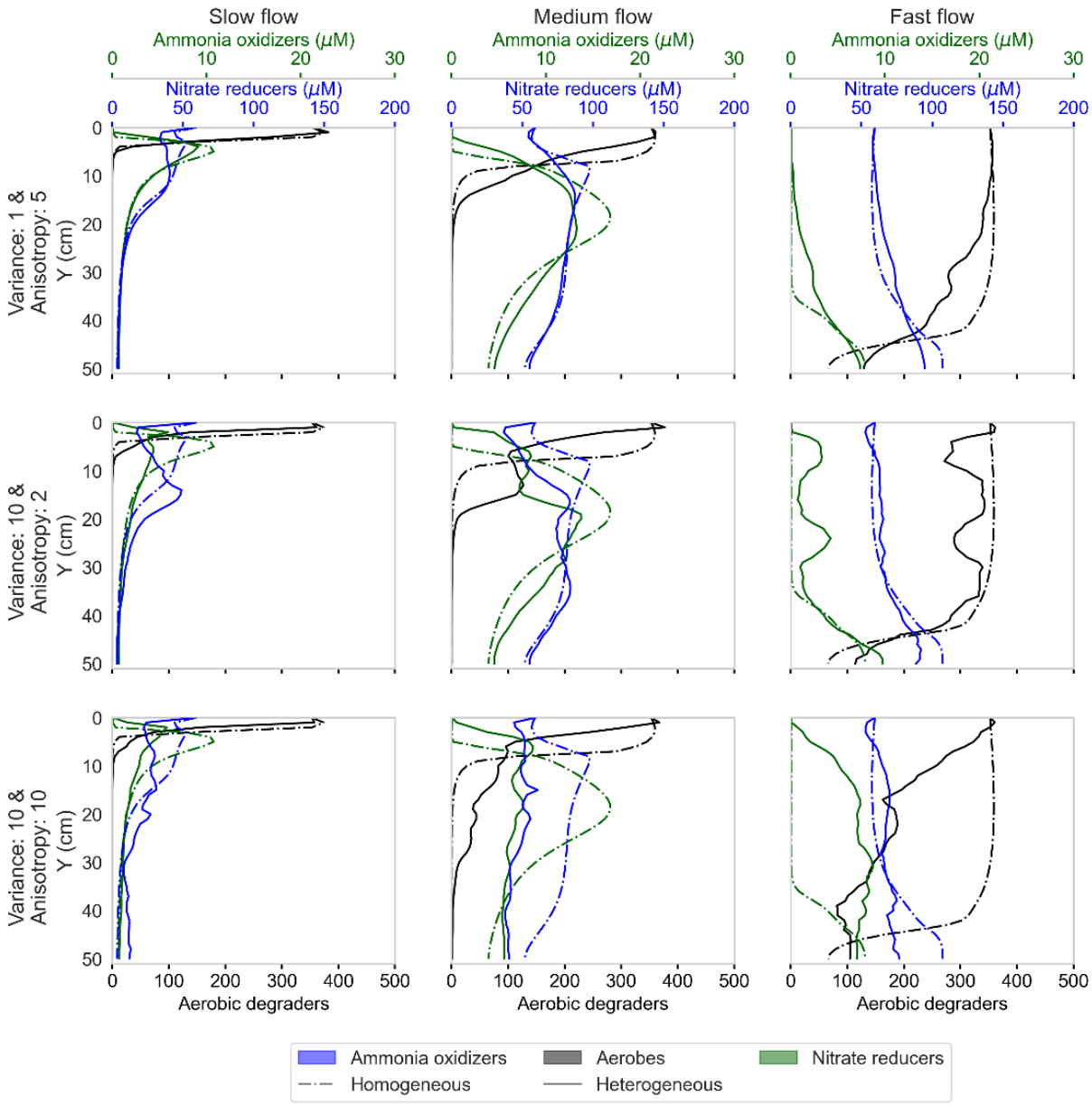


Figure S2: Spatially averaged concentration profile of the immobile active biomass in heterogeneous domains (indicated by variance and anisotropy values in the row index) in three types of heterogeneous scenarios (solid lines) compared to that in the homogeneous base case (zero variance and no associated anisotropy, dashed-dot lines) in all flow regimes. The spatially averaged concentration profile is the same for a given column (i.e., there is only one homogeneous/base case for comparison in each flow regime).

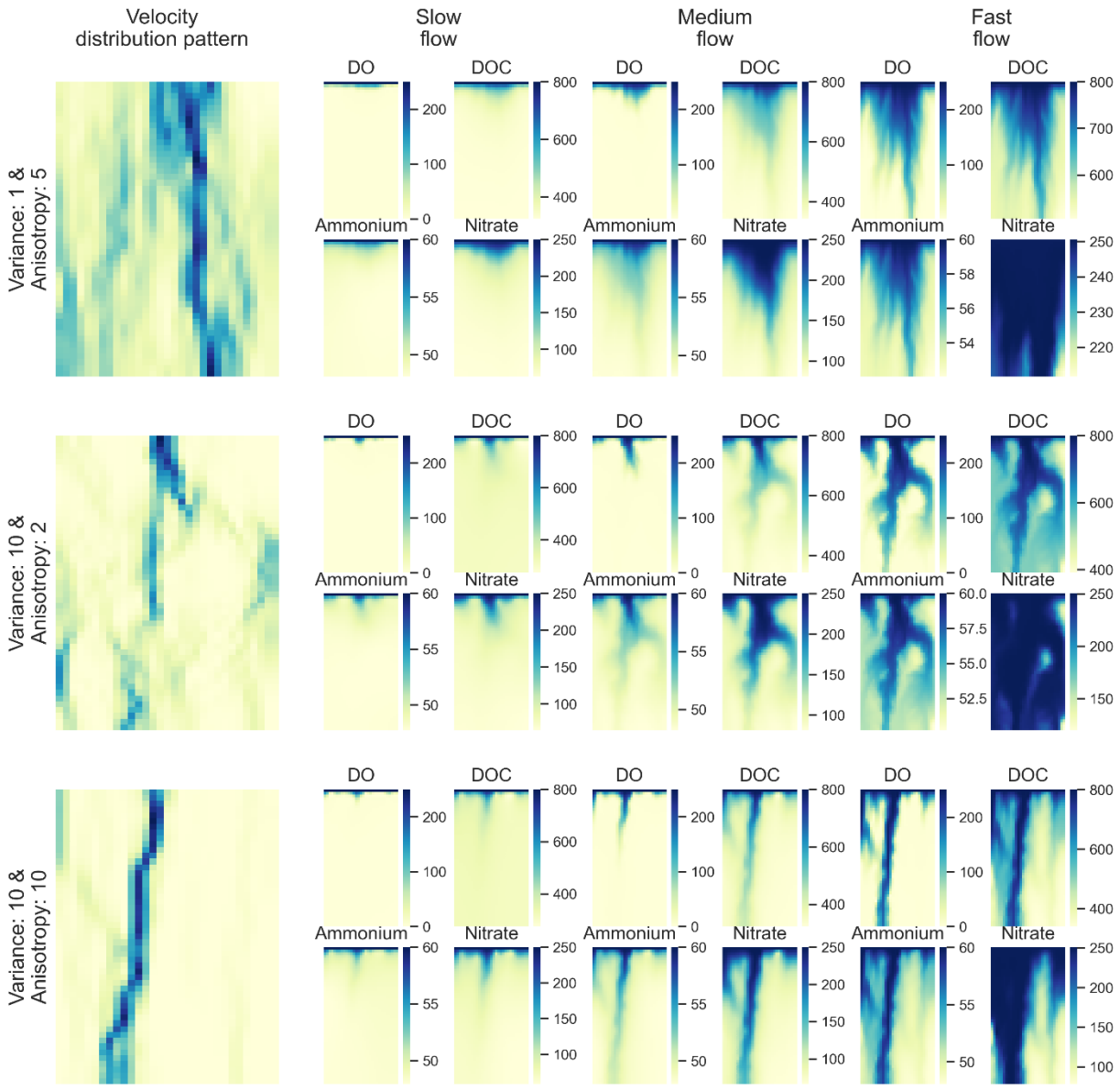


Figure S3: 2D concentration distributions of dissolved species in heterogeneous domains (µM) with the velocity distribution (in m d^{-1}) in these domains.

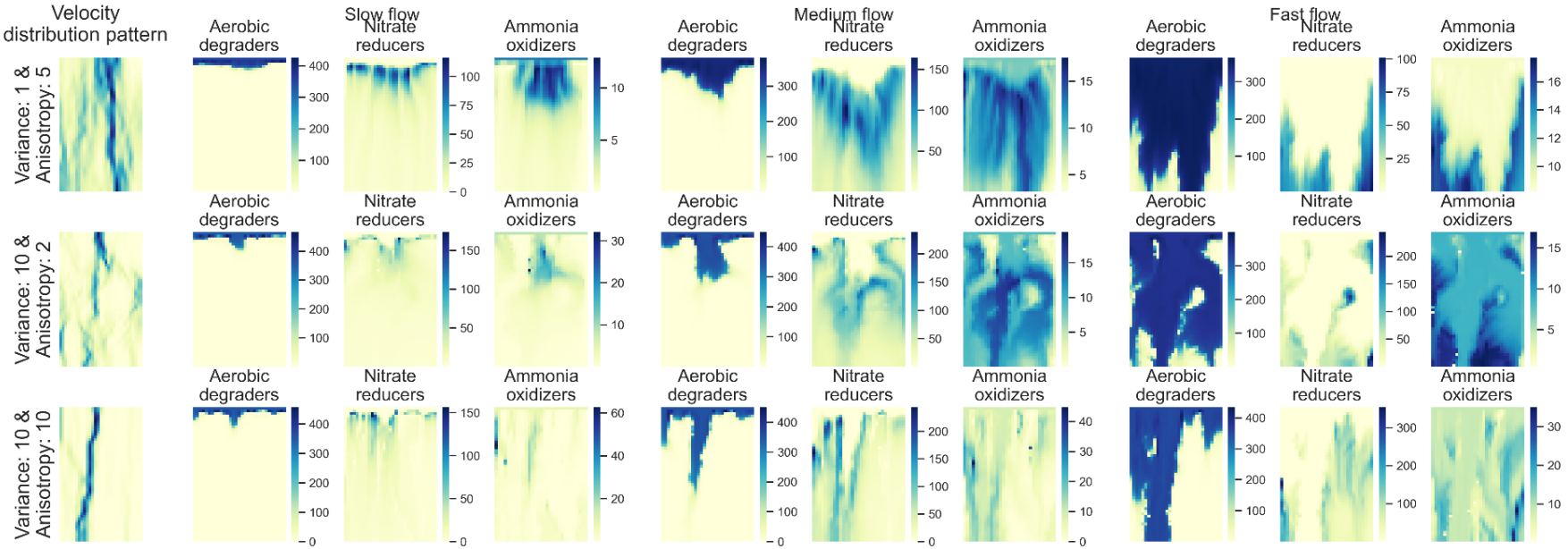


Figure S4: 2D concentration distributions of microbial species in heterogeneous domains (μM) with the velocity distribution (in m d^{-1}) in these domains

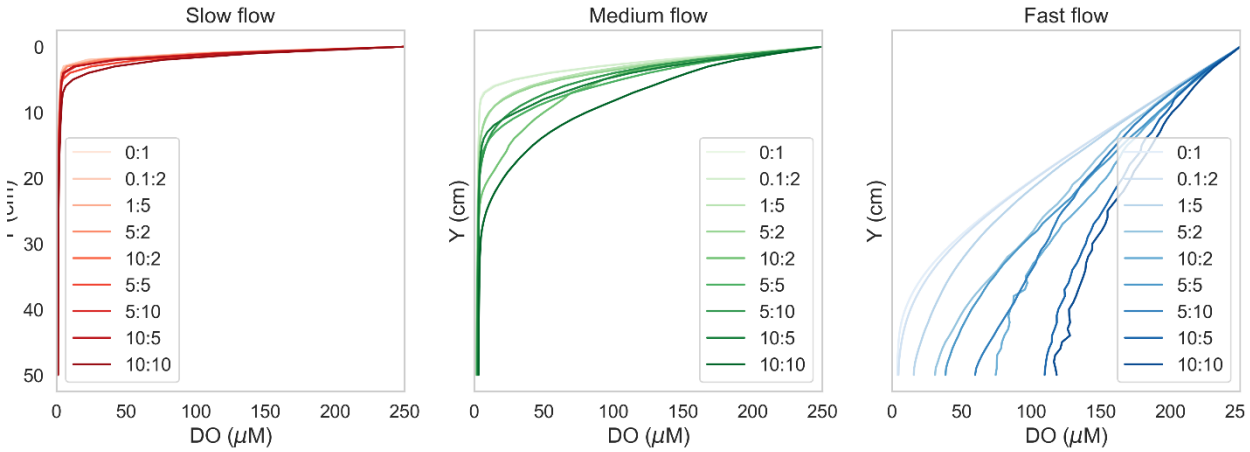
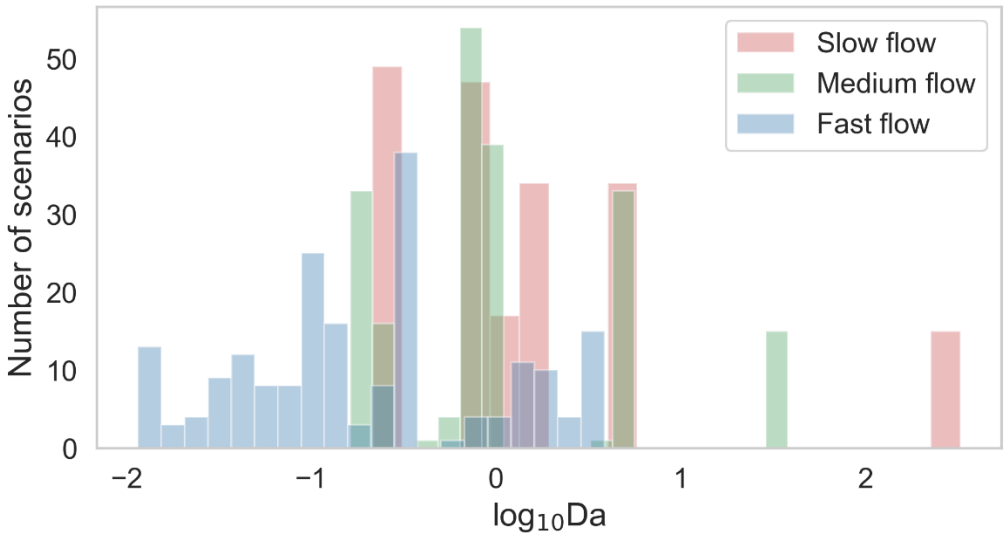


Figure S5: Increasing DO persistence with heterogeneity (presented in the legend as Variance in permeability field: Anisotropy)

(a)



(b)

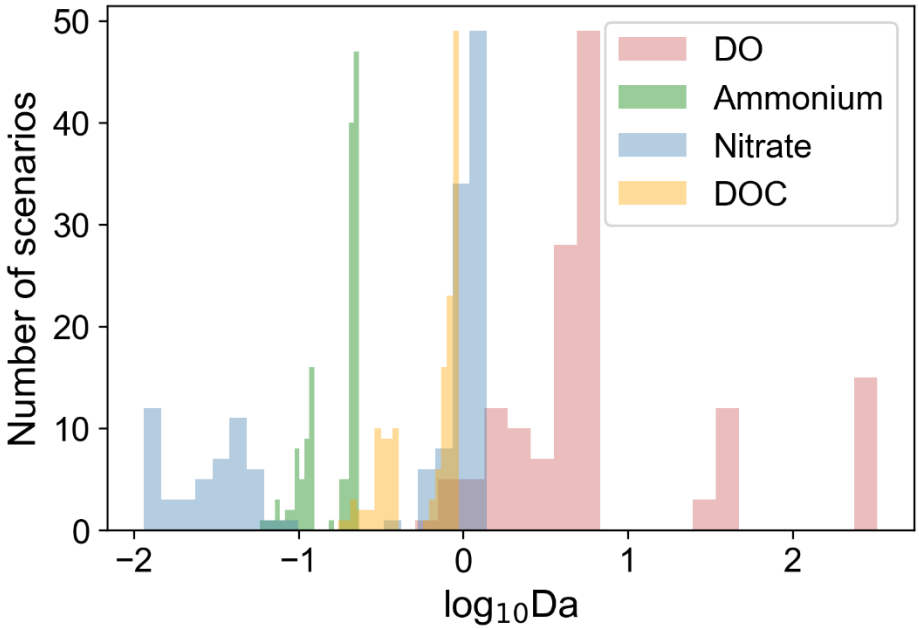


Figure S6: Distribution of Damköhler number (Da) in the investigated scenarios. Panel (a) presents the Da of all chemical species in all domains, differentiated by the flow regime: Slow flow regime is in red, medium flow regime is in green, and fast flow regime is in blue). Panel (b) presents the Da of all chemical species in all domains, differentiated by the chemical species: DO is in red, ammonium is in green, nitrate is in blue and DOC is in orange.

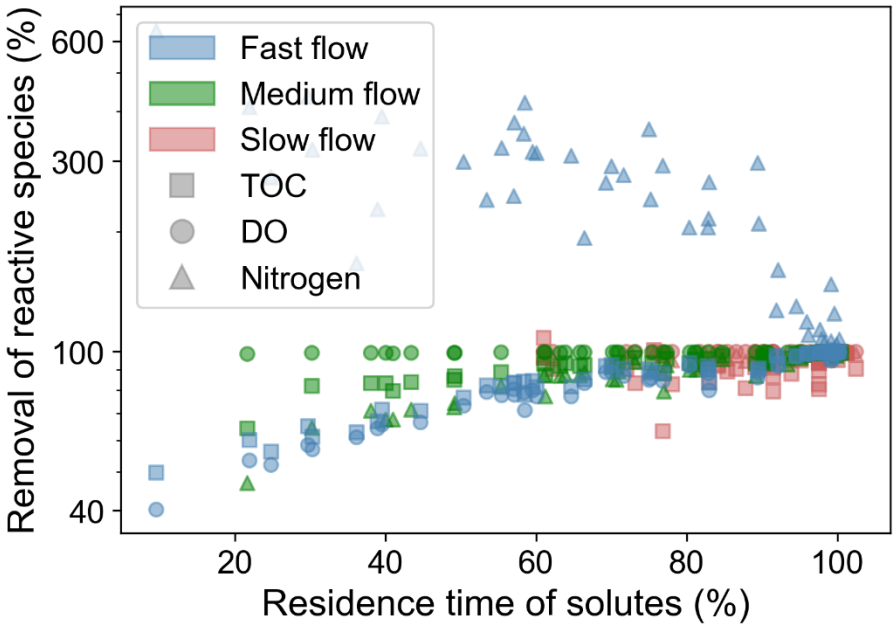


Figure S7: Impact on (normalized) removal of reactive species as a result of spatial heterogeneity characterized as reduction in solute residence times in the domain

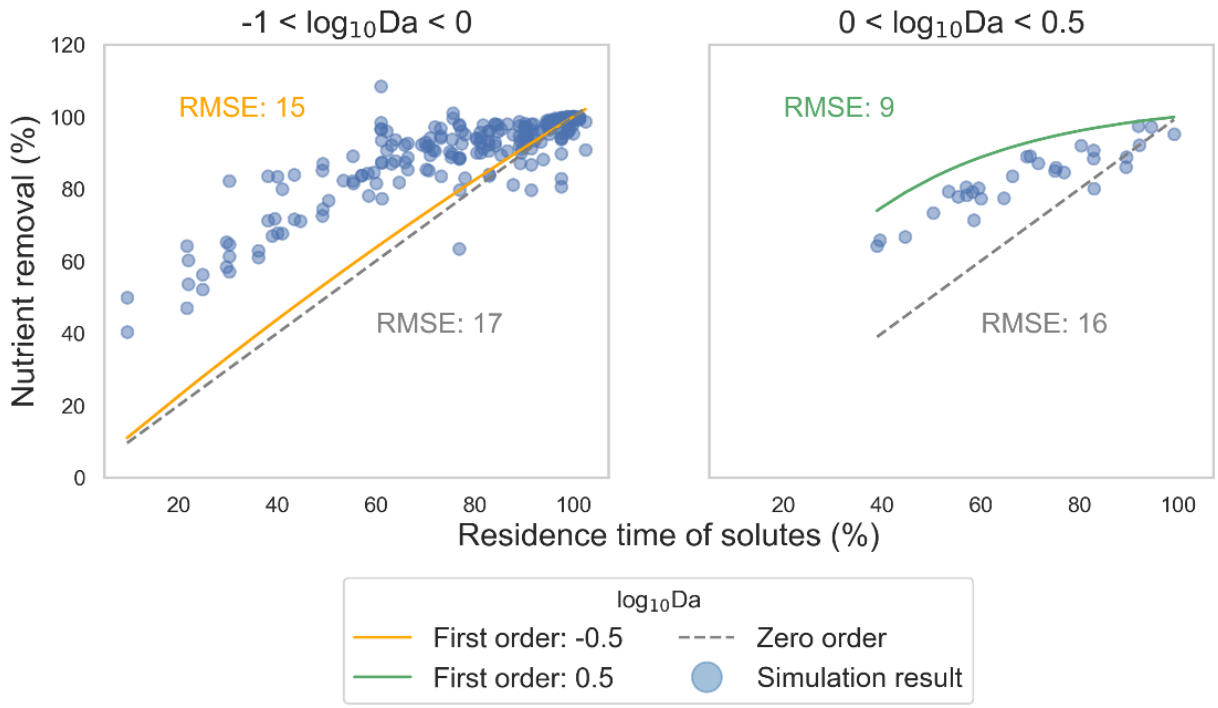


Figure S8: Comparison of simulation results and corresponding analytical solutions for changing removal of reactive species with changing residence time alone.

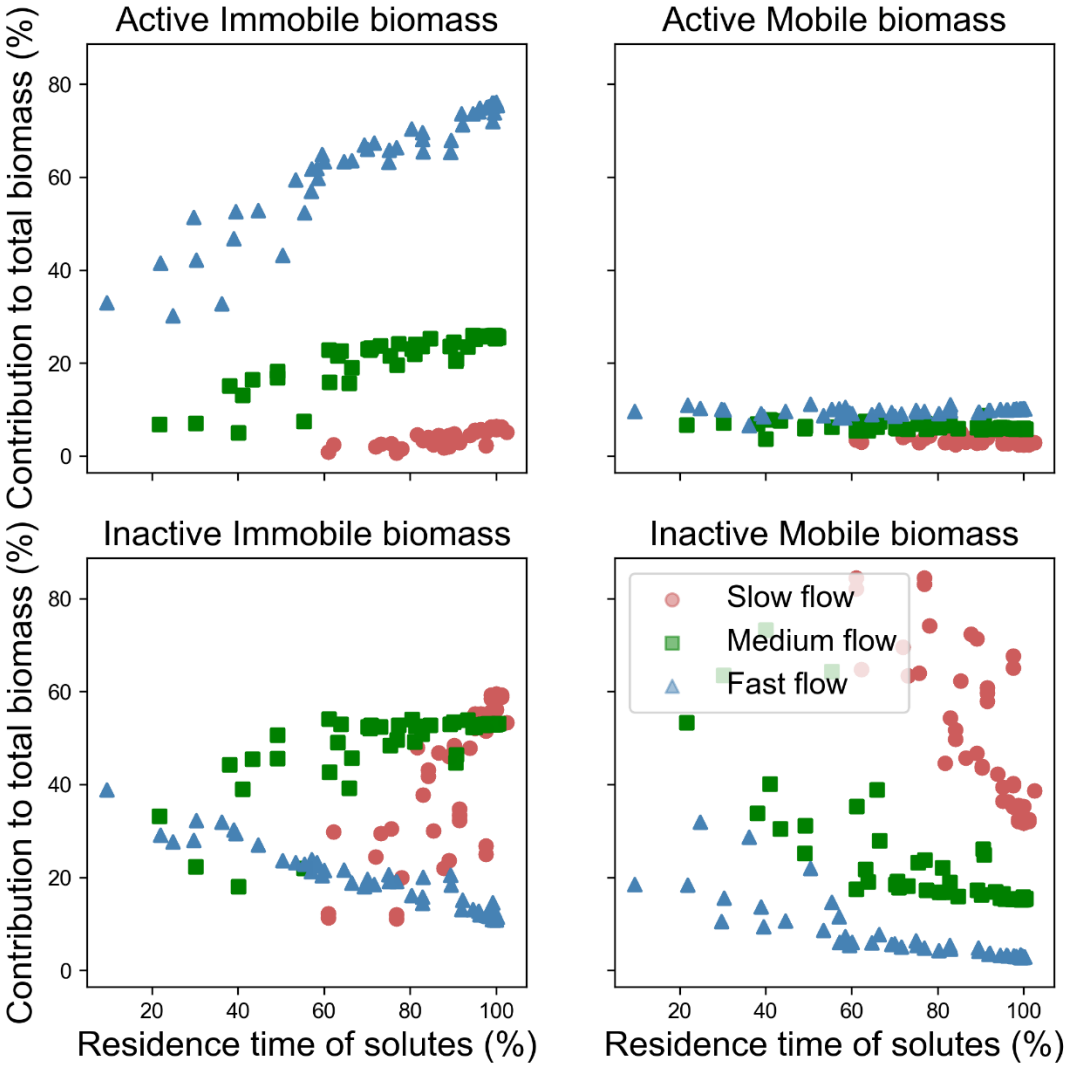


Figure S9: Contribution to total biomass of different fractions of microbial species with increasing spatial heterogeneity (i.e., decreasing residence time of solutes).

Tables

Table S1 Linear mixed models for the simulation dataset

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 S2 Mixed linear effects model results: Summary

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				