

Modelling Phosphorus Sorption Kinetics and the Longevity of Reactive Filter Materials Used for On-site Wastewater Treatment

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1. Supplementary Material A: Conceptual diagram of the model

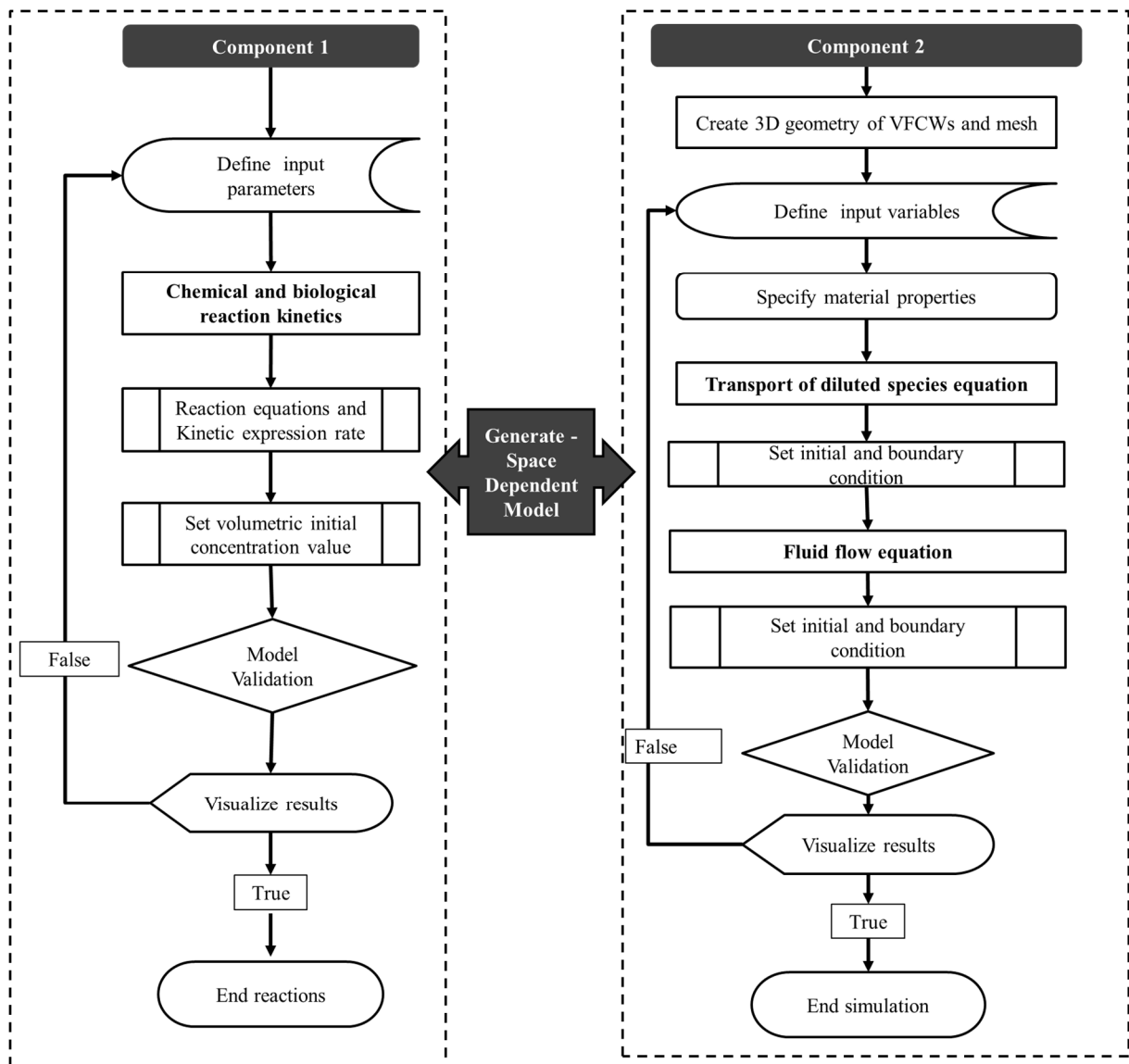


Figure A1. Conceptual diagram of the coupled kinetics and transport model implemented in COMSOL Multiphysics for predicting phosphorus (P) retention and mobility in reactive P-filters.

2. Supplementary Material B: Calcium phosphate mineral phases used in geochemical modelling

Table B1. Calcium phosphate mineral phases used in geochemical modelling of mineral precipitation and dissolution using the reference input data of solubility product constant (Ksp), ion activity product (IAP), saturated index (SI) and heat of reaction (ΔH_r)

Mineral phase	logK _{sp}	logIAP	SI	ΔH_r kJ mol ⁻¹	Process	Reference
HAP: $5\text{Ca}^{2+} + 3\text{PO}_4^{3-} + \text{H}_2\text{O} \rightleftharpoons \text{Ca}_5(\text{PO}_4)_3\text{OH} + \text{H}^+$	-44.3	-43	1.3	0	Precipitation	Smith et al., 2003.
DCPD: $\text{Ca}^{2+} + \text{PO}_4^{3-} + \text{H}^+ + 2\text{H}_2\text{O} \rightleftharpoons \text{CaHPO}_4 \cdot 2\text{H}_2\text{O}$	-28.25	-19.9	8.3	-87	Precipitation	Smith et al., 2003.
OCP: $4\text{Ca}^{2+} + 3\text{PO}_4^{3-} + \text{H}^+ \rightleftharpoons \text{Ca}_4\text{H}(\text{PO}_4)_3$	-47.95	-40.5	7.5	-105	Precipitation	Christoffersen et al., 1990
ACP: $3\text{Ca}^{2+} + 2\text{PO}_4^{3-} \rightleftharpoons \text{Ca}_3(\text{PO}_4)_2$	-25.5	-25.3	0.2	-94	Precipitation	Christoffersen et al., 1990
DCP: $\text{Ca}^{2+} + \text{HPO}_4^{2-} \rightleftharpoons \text{CaHPO}_4$	-19.28	-11.9	7.4	31	Precipitation	Smith et al., 2003.
Calcite: $\text{CaCO}_3 + 2\text{H}^+ \rightleftharpoons \text{Ca}^{2+} + \text{CO}_2 + \text{H}_2\text{O}$	-8.48	-5.43	3.1	-9.6	Dissolution	Parkhurst and Appelo.,2011

Abbreviations: **HAP:** Hydroxyapatite; **ACP:** Amorphous calcium phosphate; **DCP:** Dicalcium phosphate; **DCPD:** Diabasicdicalcium phosphate; **OCP:** Octacalcium phosphate

3. Supplementary Material C: Reference data used for calibrating the model

Table C1. Parameters adjusted fit simulation results to the observed data.

Parameter	Unit	Filtralite P	Polonite	Top16
<i>Hydraulic parameter</i>				
Mean particle size	[mm]	5.6	4.3	6
Porosity, $\emptyset$	[-]	0.65	0.56	0.57
Hydraulic conductivity, K	[m/d]	100	800	500
Bulk density, ρ_b	[kg/m ³]	500	781	745
Gravity acceleration, g	[m/s ³]		9.81	
Dynamic water viscosity, μ_w	[Pa*s]		8.43*10 ⁻⁴	
Hydraulic loading rate (HLR)	[L/(d*m ²)]		850	
<i>Reactive transport and adsorption parameter</i>				
PO ₄ -P influent concentration	[mg/l]	11.4 ± 1.3	11.9 ± 1.2	11.0 ± 1.2
Total-P influent concentration	[mg/l]	11.4 ± 1.4	12.1 ± 1.2	12.0 ± 1.5
Total Organic Carbon (TOC) influent concentration	[mg/l]	130 ± 3	22.2 ± 5.3	22.1 ± 5.7
pH of virgin reactive media	[-]	10.6	13	10.5
pH of influent wastewater	[-]	9.6 ± 0.6	7.3 ± 0.4	7.6 ± 0.2
Redox potential	[mV]	222.2 ± 31.5	191 ± 37	
Molecular Diffusion coefficient, D _m	[m ² /s]		1.295*10 ⁻⁹	
Longitudinal dispersity, α_L	[m]		2.5*10 ⁻³	
Transverse dispersity, α_T	[m]		3.3*10 ⁻³	
<i>Final parameters fitted to the observed data</i>				
Permeability	[m ²]	1.093*10 ⁻¹⁰	9.949*10 ⁻¹⁰	1.002*10 ⁻⁹
Hydrolysis rate coefficient, K _h	[1/day]	2.3	3.1	2.8
Adsorption isotherm coefficient, K _L	[L/kg]	41.13	55.54	30.70
Langmuir adsorption capacity, b	[(g/kg)]	4.3	6.8	5.5

4. Supplementary Material E: Change in spatial distribution of phosphorus (P) sorption in the current design of P-filter bag.

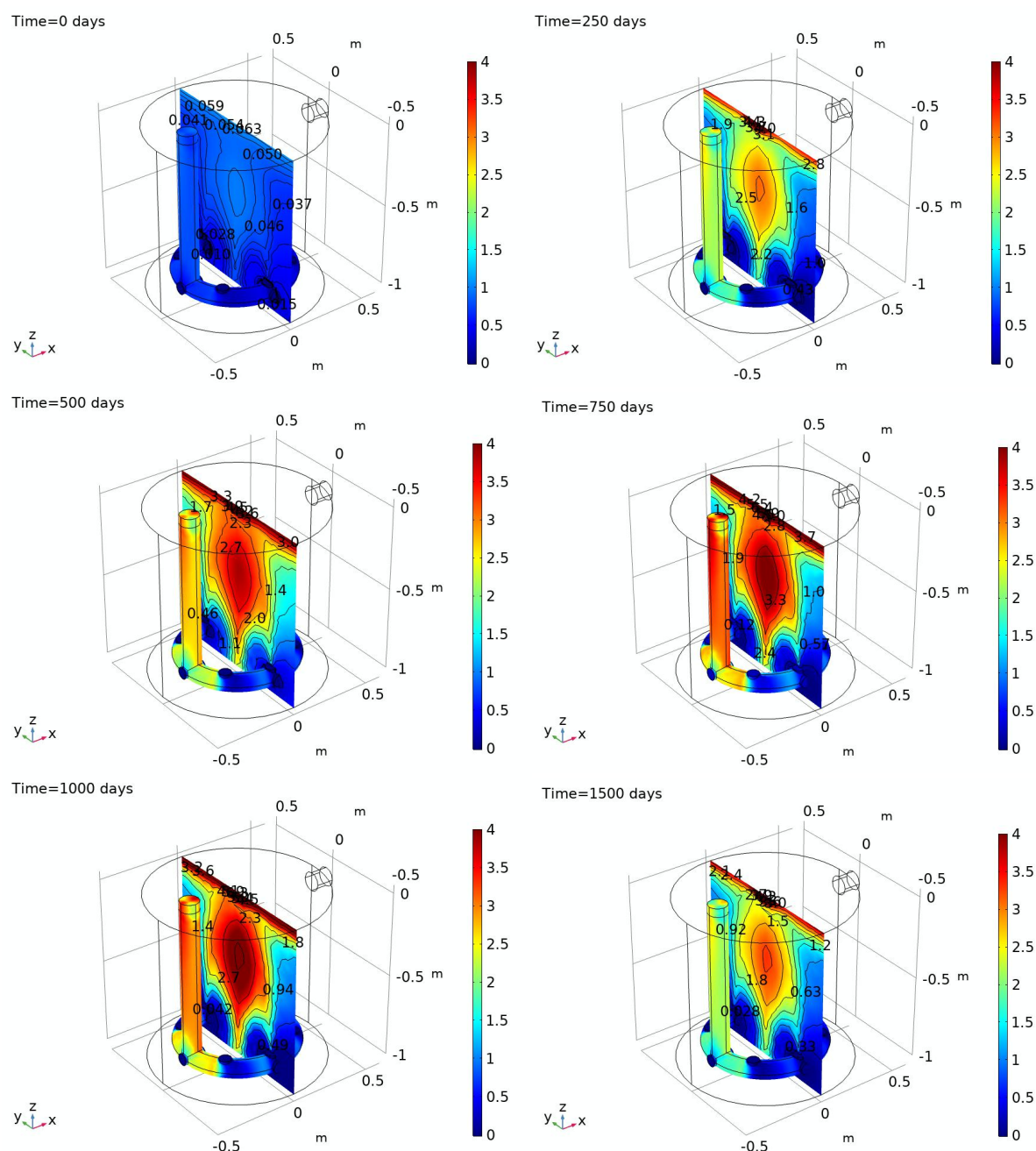


Figure E1. Change in spatial distribution of phosphorus (P) sorption in the current design of P-filter bag (circular distribution pipe) with different simulated operating times from 0 to 1500 days.

5. Supplementary Material F: Change in spatial distribution of phosphorus (P) sorption in the modified P-filter bag.

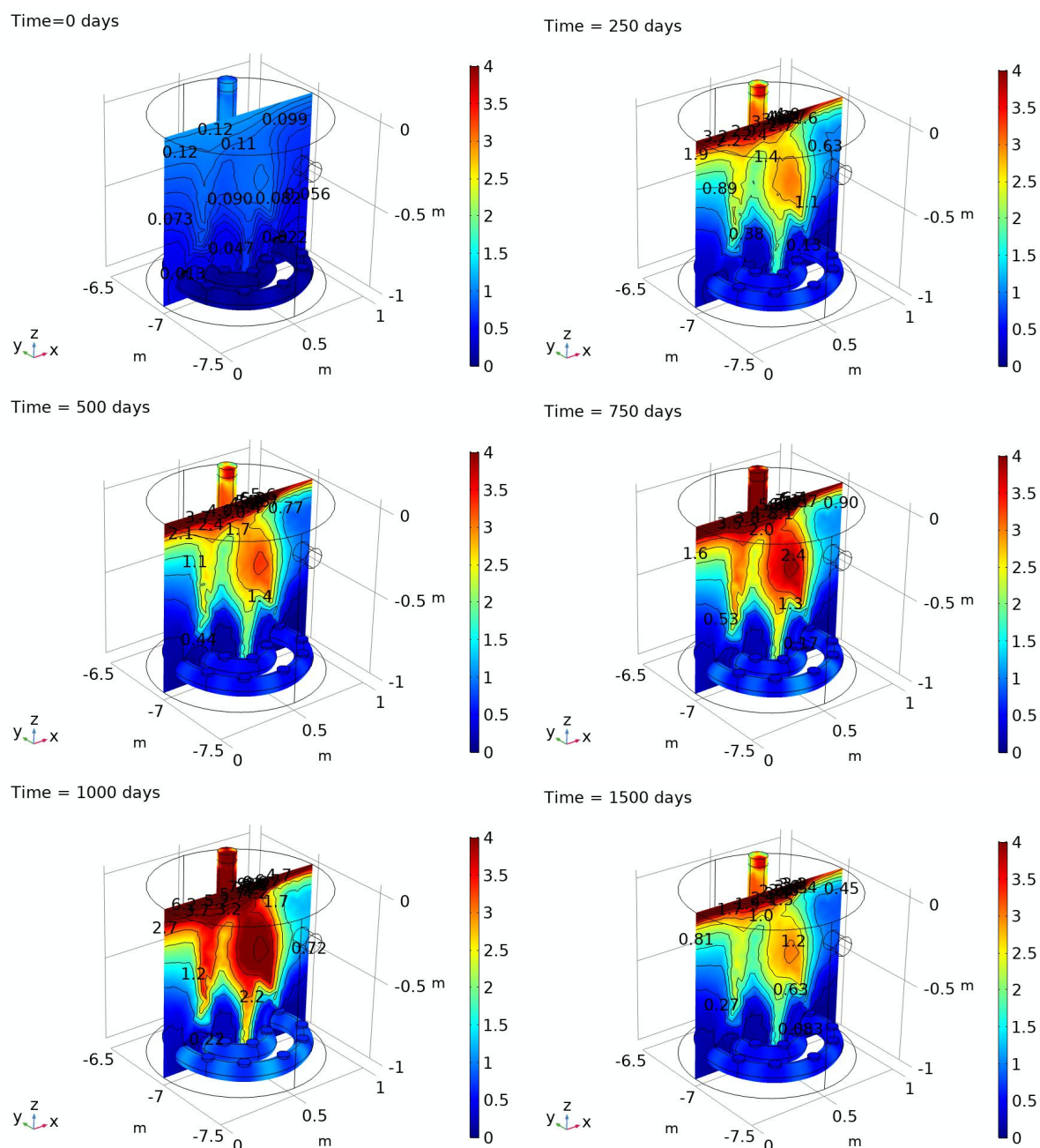


Figure F1. Change in spatial distribution of phosphorus sorption in the modified P-filter bag (spiral distribution pipe) with different simulated operating times from 0 to 1500 days.