

Supplementary file S1– Supplementary tables and figures

Matteo Antelmi¹, Pietro Mazzon^{1*}, Patrick Höhener², Massimo Marchesi¹, Luca Alberti¹

¹ Politecnico di Milano, Civil and Environmental Engineering Department (DICA), P.zza L. da Vinci 32, 20133 Milano, Italia.

² Aix-Marseille Université - CNRS, UMR 7376 Laboratory of Environmental Chemistry

* Corresponding author: Tel. +39 02 2399 6668, pietro.mazzon@polimi.it

Attached to the paper there are 3 other Annexes: Annex B, Annex C and Annex D.

Supplementary tables and figures

This appendix introduces supplementary figures and tables, along with short descriptions.

Table S1 – Model parameters for the synthetic case

Parameter	Symbol	Value	Unit
Domain length	L	500	m
Total simulation time	-	30	years
Average pore water velocity	v_r	3.47×10^{-6}	m/s
Retardation factor ¹	R_f	2.14	-
Longitudinal dispersivity	α_L	20	m
Transversal and vertical dispersivity	$\alpha_{T,V}$	0	m
Source area ²	S_a	1 x 1	m ²
Cell length ³	l	7.14	m
Cell number ³	-	70	-
Shifts ³	-	459	-
Time step length ³	TS	2056580	s
Flow direction ³	-	forward	-
Boundary conditions (BCs) ³	-	constant - flux	-
Degradation rate constant	λ	PCE	3.2×10^{-8}
		TCE	2.4×10^{-8}
		1,2-cis-DCE	1.5×10^{-8}
		VC	7×10^{-9}
Enrichment Factor	ε	PCE	-4
		TCE	-12
		1,2-cis-DCE	-20
		VC	-25

¹ Used only in Case 2; ² Only used in BIOCHLOR-ISO; ³ Only needed for PHREEQC

Table S2 – Concentration and isotopic composition of the source

Parameter	Symbol	Compound	Initial value	Unit
Source concentration	C_0	PCE	0.5	mM
		TCE	1	
		1,2-cis-DCE	0	
		VC	0	
Source isotopic composition	$\delta^{13}C_0$	PCE	-30.0	‰
		TCE	-25.0	
		1,2-cis-DCE	0	
		VC	0	

Table S3 - Initial values of the degradation rates and enrichment factors, source concentrations and isotopic compositions of the field case

Parameter	Symbol	Compound	Initial value	R ²	Retarded value ¹	Unit
Degradation rate	λ	TCE	3.197	0.96	0.855	1/yr
		1,2-cis-DCE	0.045	0.21	0.012	
		VC	3.849	0.97	1.029	
Enrichment factor	ε	TCE	-22.9	-	-	-
		1,2-cis-DCE	-30.5			
		VC	-31.2			
Input concentration	C_0	TCE	46.1	-	-	$\mu\text{g/l}$
		1,2-cis-DCE	41.8			
		VC	74.0			
Initial isotopic composition	$\delta^{13}\text{C}_0$	TCE	-67.1	-	-	-
		1,2-cis-DCE	-58.9			
		VC	-57.6			

¹ For an overall retardation factor $R_{d,model} = 3.74$ **Table S4** - Partition coefficients, retardation factors and average retardation factor for the compounds of interest

Compound	$k_{oc} [\text{cm}^3/\text{g}]$	$R_d [-]$	$R_{d,model} [-]$
TCE	130	4.76	3.74
1,2-cis-DCE	125	4.61	
VC	29.6	1.86	

Table S5. Statistical analysis of the enrichment factor database

Statistic	TCE			1,2-cis-DCE			VC		
	Total	Aerobic	Anaerobic	Total	Aerobic	Anaerobic	Total	Aerobic	Anaerobic
Mean	-12.22	-11.03	-12.36	-16.07	-8.07	-20.08	-14.83	-6.10	-24.68
Median	-12.20	-11.60	-12.20	-17.25	-8.35	-18.85	-7.90	-6.40	-24.00
Std. Dev	6.34	6.09	6.39	8.00	6.17	5.39	9.60	1.37	2.92
Min	-26.60	-19.50	-26.6	-30.5	-19.90	-30.5	-31.10	-8.20	-31.10
Max	-1.10	-1.10	-2.50	-0.90	-0.90	-9.10	-3.20	-3.20	-19.90
Range	25.50	18.40	24.10	29.60	19.00	21.40	27.90	5.00	11.20
25° percentile	-15.30	-14.55	-16.05	-21.23	-11.15	-24.45	-23.85	-7.20	-26.60
75° percentile	-7.10	-6.38	-7.10	-9.03	-1.18	-16.30	-6.35	-5.40	-22.70
IQR ¹	8.2	8.18	8.95	12.20	9.98	8.15	17.78	1.80	3.90

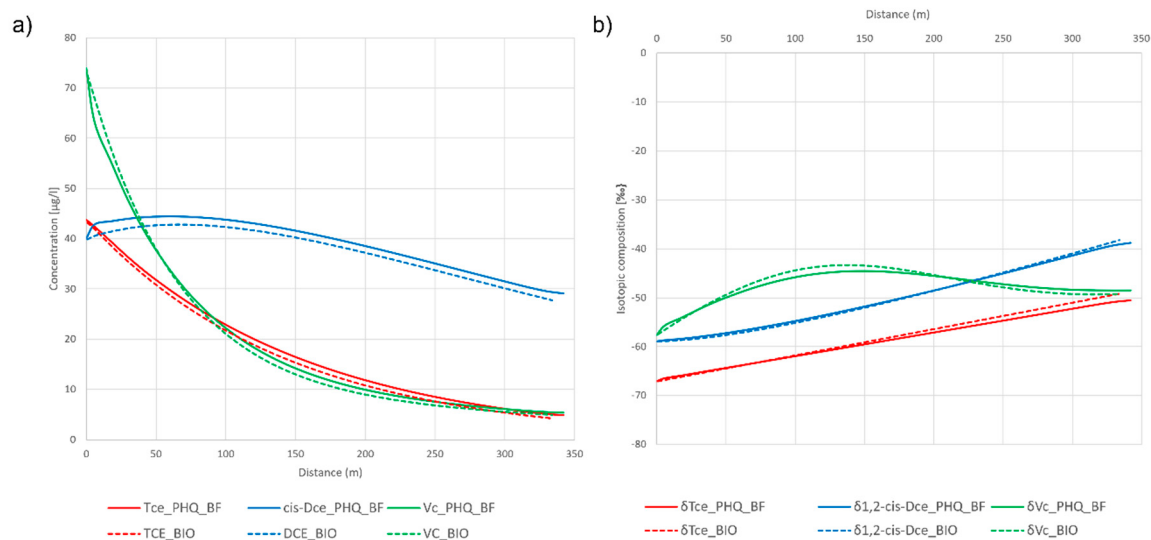


Figure S1 – Comparison between the PHREEQC solution (full line) and the BIOCHLOR-ISO solution (dashed line) in the Best Fit parameters case

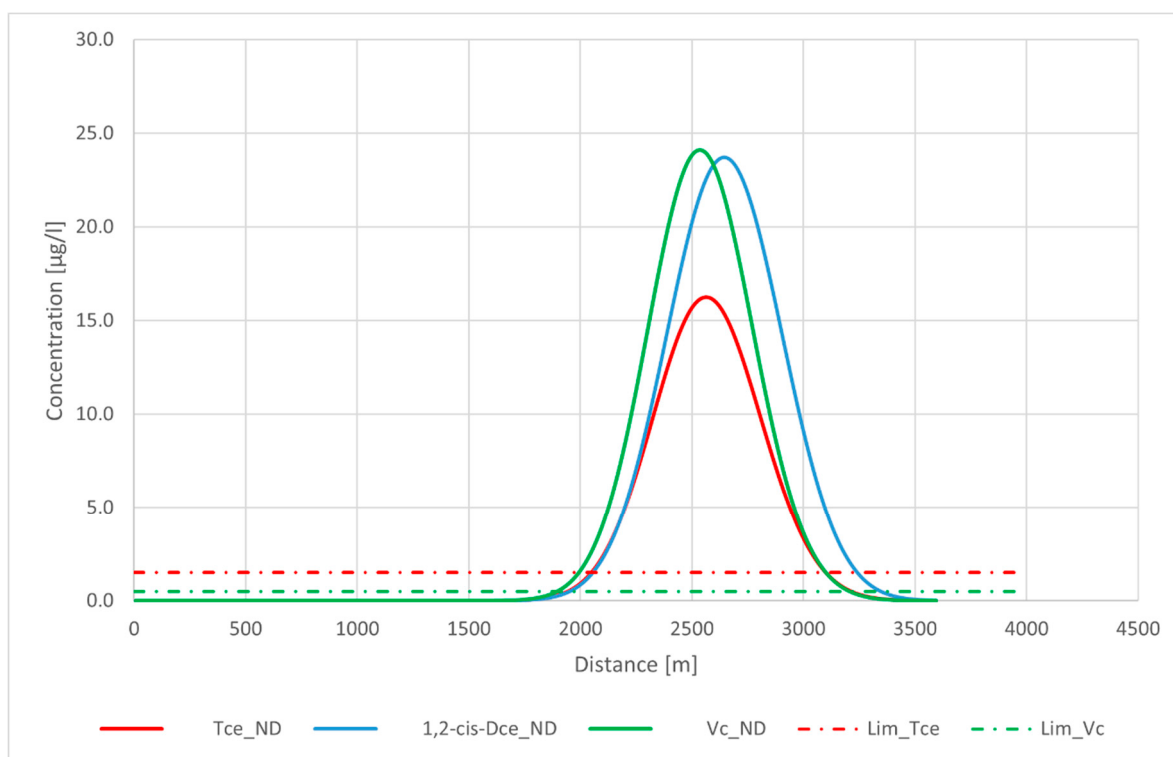


Figure S2 - Forecast model result for 30 years in the non-degradative (ND) case