

Modeling BTEX Multiphase Partitioning with Soil Vapor Extraction under Groundwater Table Fluctuation Using the TMVOC Model

Yang Yang ¹, Jingwei Zheng ², Juan Li ^{1,*}, Huan Huan ¹, Xiaobing Zhao ¹, Ningqing Lv ³, Yan Ma ² and Hao Zhang ^{1,*}

- ¹ Technical Centre for Soil, Agriculture and Rural Ecology and Environment, Ministry of Ecology and Environment, Beijing 100012, China; yangyang@tcare-mee.cn (Y.Y.); huanhuan@tcare-mee.cn (H.H.); zhaoxiaobing@tcare-mee.cn (X.Z.)
² School of Chemical and Environmental Engineering, China University of Mining and Technology (Beijing), Beijing 100083, China; zjwljwater@foxmail.com (J.Z.); mayan2202@163.com (Y.M.)
³ Chinese Research Academy of Environmental Sciences, Beijing 100012, China; lvnq@craes.org.cn
* Correspondence: lijuan@tcare-mee.cn (J.L.); zhanghao@tcare-mee.cn (H.Z.)

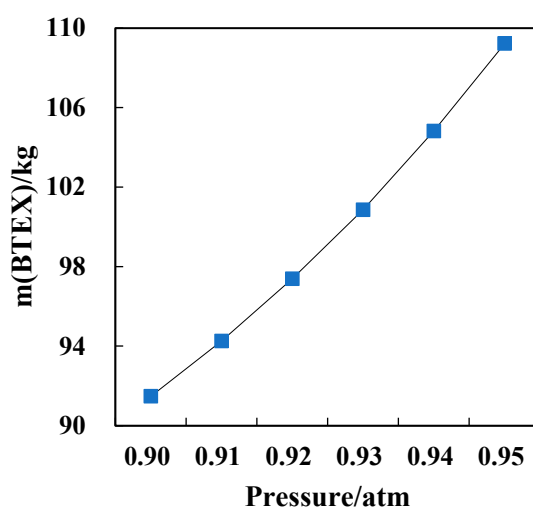


Figure S1. Masses of residual BETX after 10-day SVE at different extraction well pressures

Table S1. Main petrophysical properties of rock domains

Sample	Lithology	Rock grain density (kg/m ³)	Porosity	Horizontal penetration rate (m ²)	Vertical penetration rate (m ²)	Ref.
1	Sand	2700	0.30	4×10^{-11}	2×10^{-11}	Battistelli, 2008
2	Sandy loam	2700	0.33	1×10^{-11}	1×10^{-12}	

Table S2. Mesh of the conceptual model

Row					Column								
Row/ column	1	2-45	46- 53	54- 57	1	2	3	4-6	7-15	16- 20	21- 22	23	24
Distance (m)	0.001	0.05	0.1	0.5	0.001	10	5	2	1	2	5	10	0.001

Table S3. Water injection/extraction parameters in the simulation area

Period	Injection			Extraction		
	Apr-Sep			Oct-Mar		
Boundary grid	1-4	5-12	13-20	58-61	62-69	70
Flow rate (kg/s)	1.9532×10^{-4}	3.9064×10^{-5}	1.9532×10^{-6}	1.9532×10^{-4}	3.9064×10^{-5}	1.9532×10^{-6}

Table S4. Average GT depth at monitoring wells for Scenario 3

GTF trend	Period	Initial GT depth in the model (m)	GT depth after the change in the model (m)	Initial GT depth in actual monitoring well (m)	GT depth after the change in actual monitoring well (m)
Descend	January–March (0–90 d)	1.825	2.75	1.80	2.50
Ascend	April–September (90–270 d)	2.75	2.40	2.50	2.00
Descend	October–December (270–360 d)	2.40	2.8	2.00	2.50

Table S5. Compositions of leaked BTEX and properties of different components

Chemicals	Formula	Relative density (water=1)	Molecular weight	Boiling point (°C)	Solubility/(mg/L) at 25°C	Henry constant
Benzene	C ₆ H ₆	0.879	78.11	80.10	1791	0.226
Toluene	C ₇ H ₈	0.857	92.14	110.63	535	0.270
Ethylbenzene	C ₈ H ₁₀	0.867	106.16	136.20	161	0.322
o-xylene	C ₈ H ₁₀	0.880	106.16	144.40	178	0.173

Table S6. Location of the extraction well

Extraction well	X/m	Y/m	Z/m
W1	22	0.5	-0.5 -1.7
W2	37	0.5	-1.0 -1.7
W3	53	0.5	-1.0 -1.85

Reference

Battistelli, A. Modeling Multiphase Organic Spills in Coastal Sites with TMVOC V.2.0[J]. Vadose Zone Journal, 2008, 7(1):316-324.