**Supplementary Material**

# Modeling solid-phase microextraction of volatile organic compounds by porous coatings using finite element analysis

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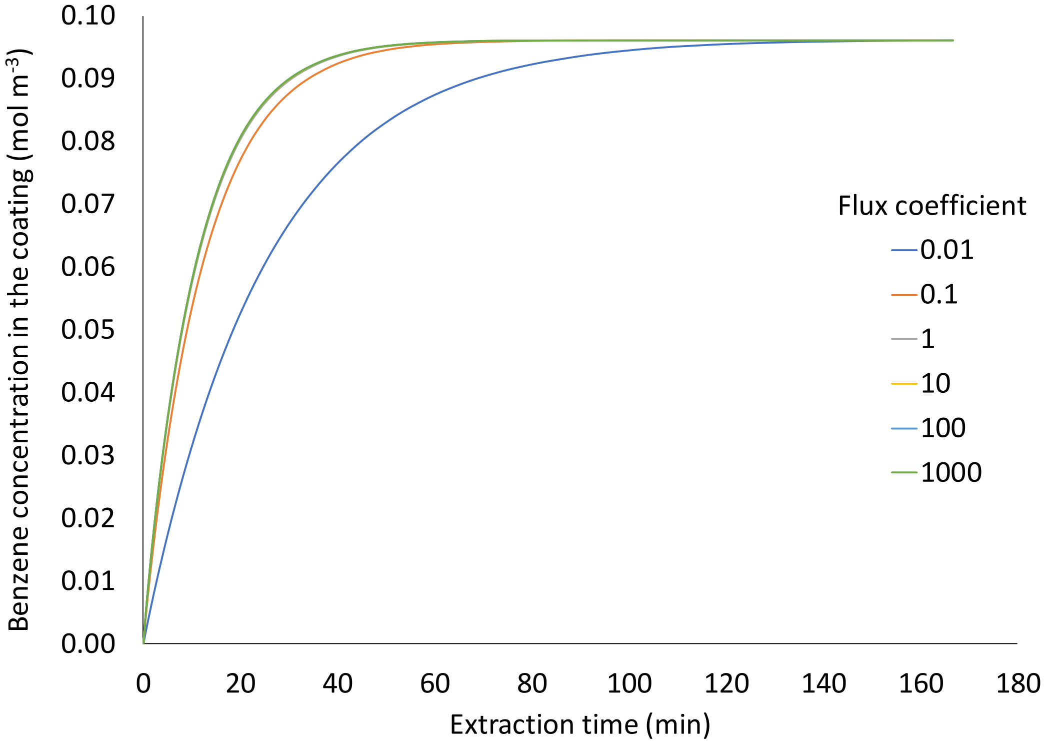


**Fig. A.1** Benzene extraction profiles from air with Carboxen/PDMS fiber obtained using 'Transport of Diluted Species' physics and different flux coefficients (*k*). Note: apparent benzene diffusion coefficient in the coating = $10^{-11}$ $m^2$ $s^{-1}$.

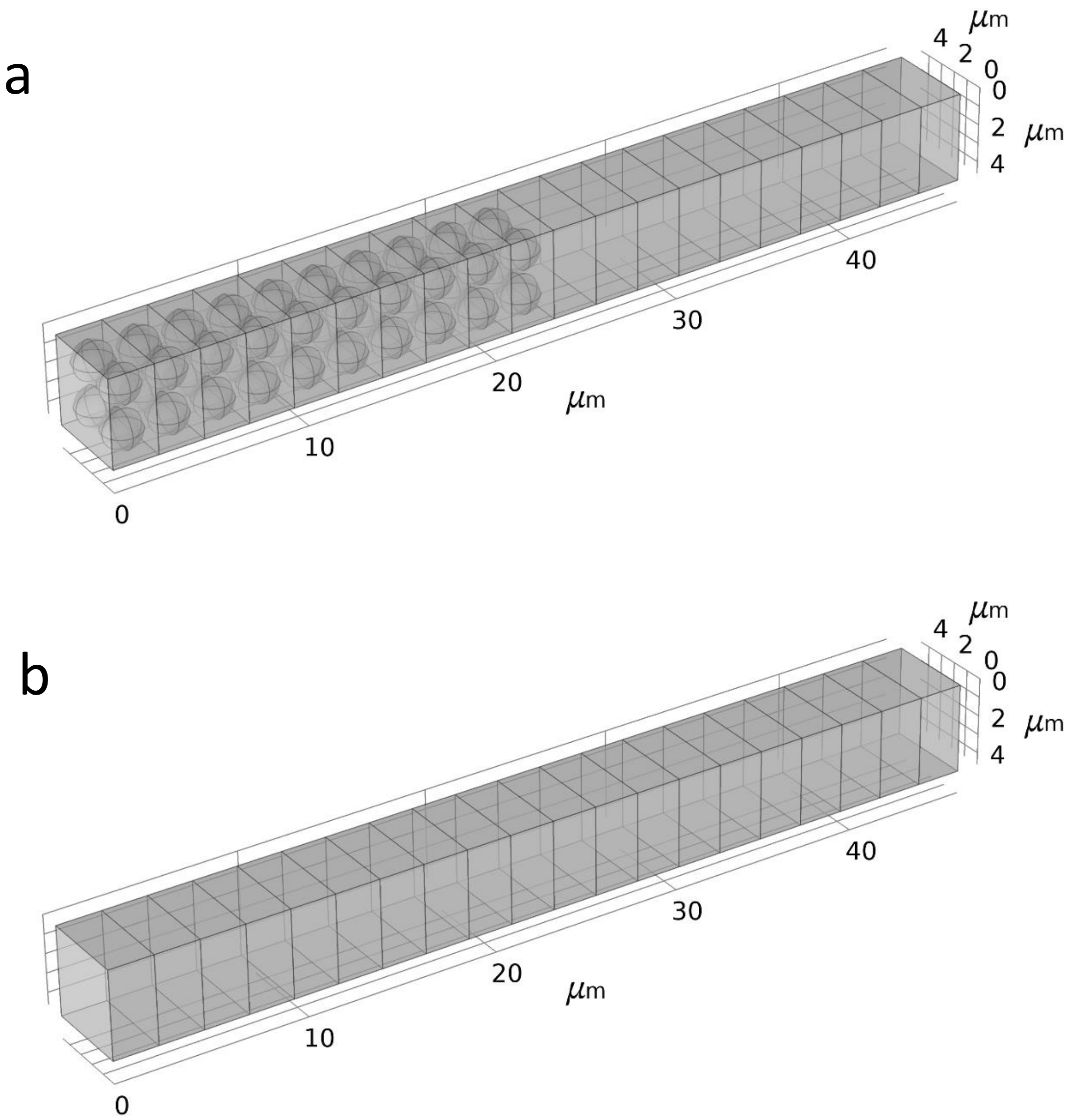


**Fig. A.2** Three-dimensional geometries with particles (a) and without particles (b) used to study mass transport of benzene in a cuboid of Car/PDMS coating. *Note:* Ten small blocks from the right side represent air; ten small blocks from the left side represent the ‘slice' of coating. Constant benzene concentration of 0.641 μmol $m^{-3}$ was set at the right edge of the geometry. Initial concentrations in the remaining parts of the geometry was set to zero.

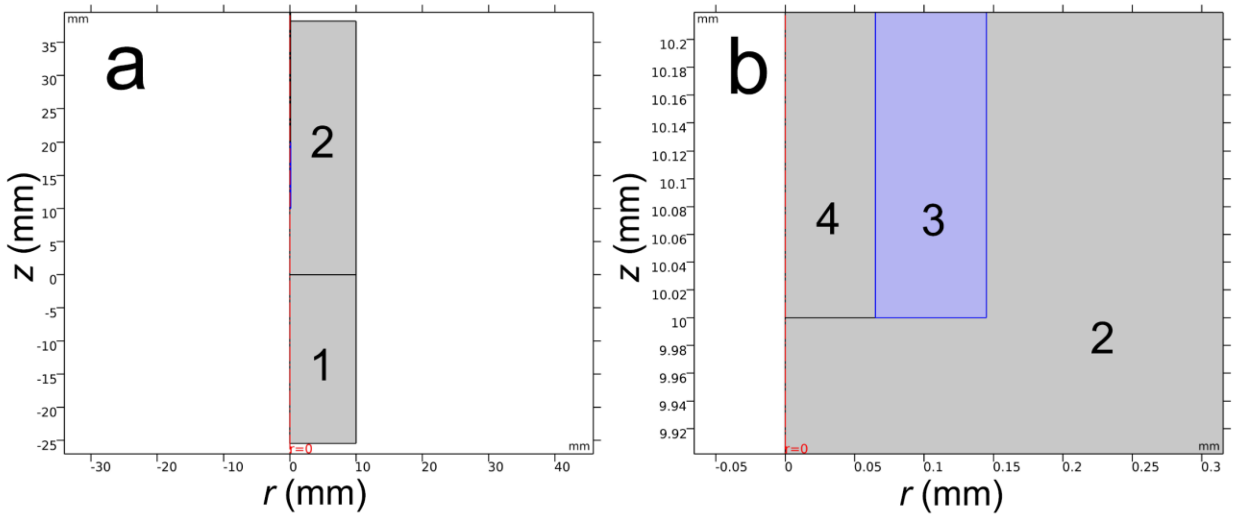


**Fig. A.3** Geometry used to model extraction of benzene from water by exposed Car/PDMS fiber. *Note:* a – full-scale geometry; b – magnified fiber tip; 1 – water sample with initial benzene concentration 0.641 mmol m$^{-3}$; 2 – headspace above water sample ($C_0$ = 0 mol m$^{-3}$); 3 – coating; 4 – fiber core.

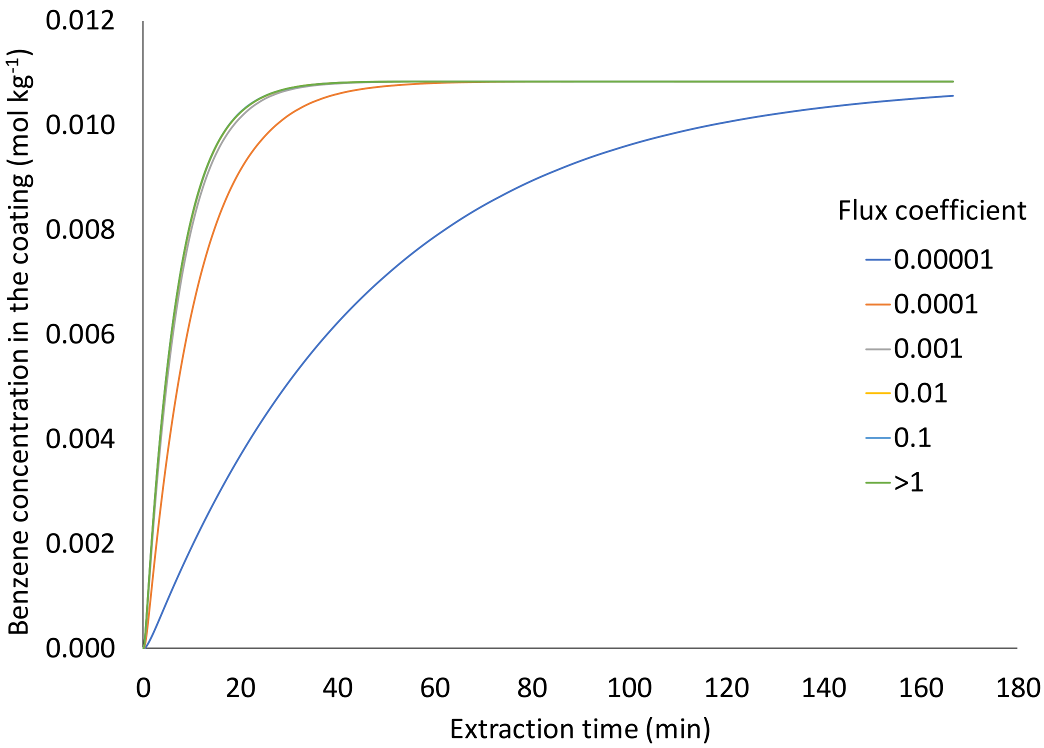


**Fig. A.4** Benzene extraction profiles from headspace above 12-mL water sample with Carboxen/PDMS fiber obtained using different water-headspace flux coefficients ($k$). Note: HLC = 0.227.

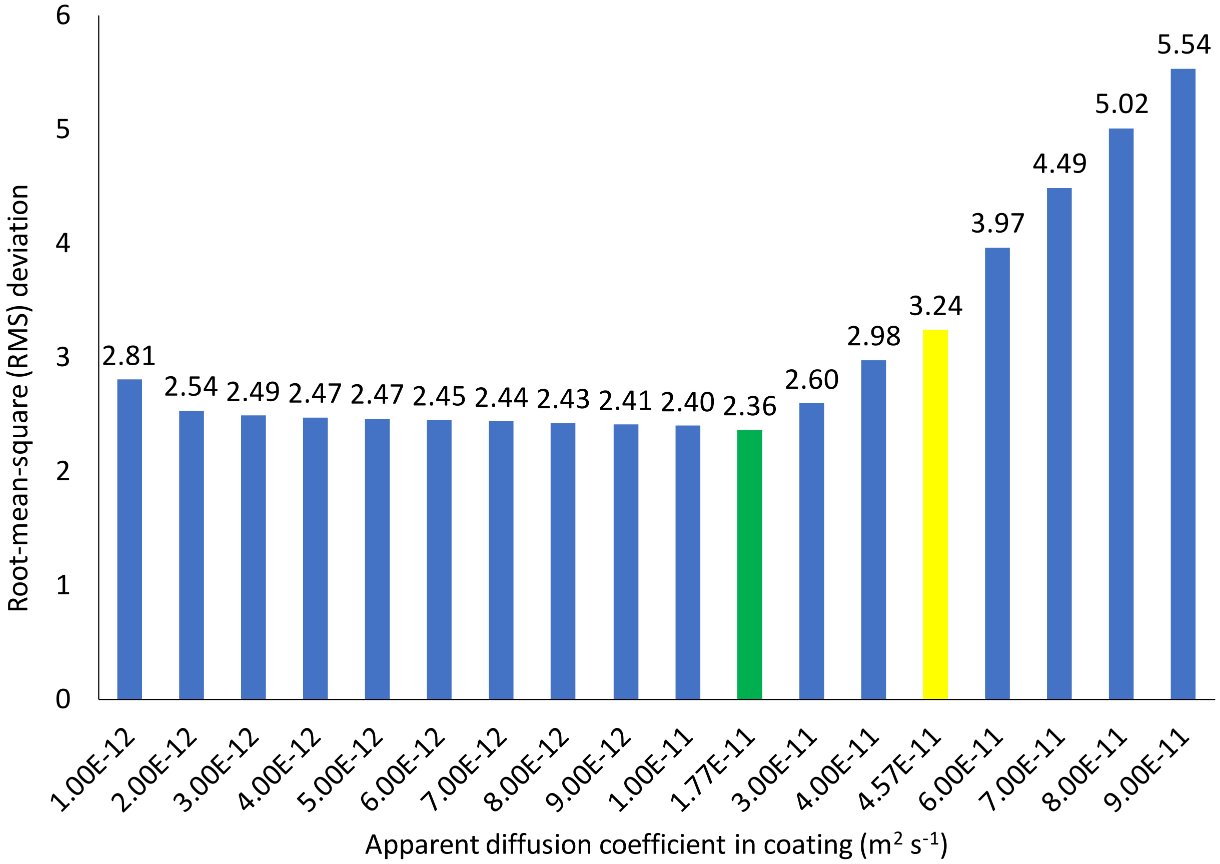


**Fig. A.5** RMS deviations obtained at different apparent diffusion coefficients. Notes: green bar represents the case when PDMS is considered as a solid phase; yellow bar represents the case when PDMS is considered as air.

## Modeling parameters ready for import to COMSOL Multiphysics

*For import to COMSOL Multiphysics software, these parameters should be copied to .txt file.*

**Modeling parameters for obtaining Fig. 3:**

KfaB 150000 "Dimensionless distribution constant between coating and air"

CoreD 0.13[mm] "Fiber core diameter"

CoatTh 0.08[mm] "Coating thickness"

Cini 6.41e-7[mol/m^3] "Initial benzene concentration in air"

DiffCbA 8.8E-6[m^2/s] "Diffusion coefficient in air"

FluxC 1000[m/s] "Flux coefficient"

DiffCbAcE 1e-11[m^2/s] "Apparent diffusion coefficient in coating"

VialD 20[mm] "Diameter of vial"

VialV 20[ml] "Volume of vial"

VialH VialV*4/pi/VialD^2 "Height of vial"

**Modeling parameters for obtaining Fig. 6 (geometry without particles):**

PartV .33 "Volumetric fraction of particles"

PartPor 0.37 "Porosity of particles"

PartDen 1000[kg/m^3] "Density of particles"

Kd1 Kd/CoatDen "Distribution constant between coating and air"

Kd 150000 "Dimensionless distribution constant between coating and air"

DiffCa 8.8e-6[m^2/s] "Diffusion coefficient in air"

CoatTort CoatPor+1.5*(1-CoatPor) "Coating tortuosity"

CoatPor 1-PartV+PartV*PartPor "Coating porosity"

CoatDen PartDen*PartV "Coating density"

**Modeling parameters for obtaining Fig. 7:**

DiffCa 8.8e-6[m^2/s] "Diffusion coefficient in air"

Kfa 150000 "Dimensionless distribution constant between coating and air"

PartV 0.33 "Volumetric fraction of particles"

Kfa1 Kfa/CoatDen "Distribution constant between coating and air"

PartPor 0.37 "Porosity of Particles"

PartTort PartPor+1.5*(1-PartPor) "Tortuosity Factor of Particles"

DiffCk 1.123e-7[m^2/s] "Knudsen diffusion coefficient in pores"

PartR 1E-6[m] "Radius of particles"

PartDen 1000[kg/m^3] "Density of particles"

CoatDen PartDen*PartV "Density of coating"

**Modeling parameters for obtaining Fig. 8:**

Cini 6.41e-7[mol/m^3] "Initial concentration in air"

CoatDen PartDen*(1-InterPartPor) "Coating density"

CoatPor InterPartPor+PartPor*(1-InterPartPor-PDMS) "Coating porosity"

CoatTh 0.08[mm] "Coating thickness"

CoatTort CoatPor+1.5*(1-CoatPor) "Coating tortuosity factor"

CoreD .13[mm] "Fiber core diameter"

DiffCbA 8.8E-6[m^2/s] "Diffusion coefficient in air"

DiffCbAc 8.8e-6[m^2/s] "Diffusion coefficient in air inside pores"

FiberL 10[mm] "Fiber length"

InterPartPor .24 "Inter-particle porosity"

Kfa1 KfaB/CoatDen "Distribution constant between coating and air"

KfaB 150000 "Dimensionless distribution constant between coating and air"

PartDen 1000[kg/m^3] "Density of particles"

PartPor 0.37 "Porosity of particles"

PDMS 0.42 "Fraction of PDMS"

VialD 20[mm] "Diameter of vial"

VialH VialV*4/pi/VialD^2 "Height of vial"

VialV 20[ml] "Volume of vial"

**Modeling parameters for obtaining Fig. 9:**

KfaB 150000 "Dimensionless benzene distribution constant between fiber and air"

CoreD 0.13[mm] "Diameter of fiber core"

CoatTh 0.08[mm] "Coating thickness"

PartPor 0.37 "Porosity of particles"

PartDen 1000[kg/m^3] "Density of particles"

InterPartPor 0.24 "Inter-particle porosity"

CoatPor InterPartPor+PartPor*(1-InterPartPor-PDMS) "Total coating porosity"

CoatDen PartDen*(1-InterPartPor) "Coating density"

KfaB1 KfaB/CoatDen "Benzene distribution constant between fiber and air"

CoatTort CoatPor+1.5*(1-CoatPor) "Coating tortuosity"

DiffCbA 8.8E-6[m^2/s] "Benzene diffusion coefficient in air"

VialV 20[ml] "Vial volume"

VialD 20[mm] "Vial diameter"

VialH VialV*4/pi/VialD^2 "Vial height"

FiberL 10[mm] "Fiber length"

WaterV "12 [ml]" "Water volume"

WaterH WaterV*4/pi/VialD^2 "Water height"

HSH VialH-WaterH "Headspace height"

FiberH 10[mm] "Fiber height"

HLC 0.227 "Henry's law constant"

CiniW 6.41e-7[mol/l] "Initial benzene concentration in water"

FluxC 1000[m/s] "Flux coefficient"

PDMS 0.42 "PDMS fraction"