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Simulating Transport and Adsorption of Organic Contaminants in 3D Porous Activated Carbon Block Media

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Access Business Group/Amway

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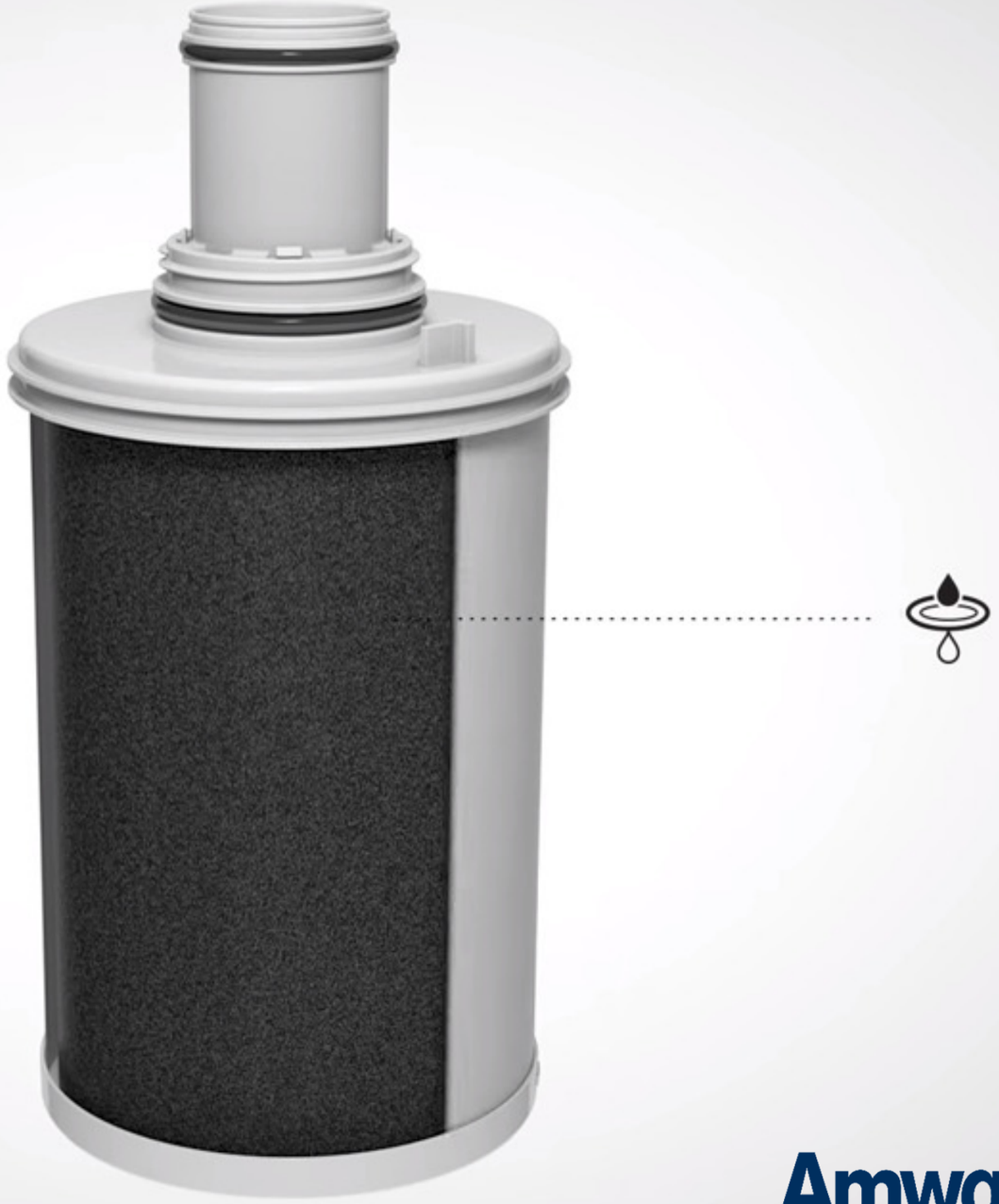
ADVANCED CARBON-BLOCK FILTER

The eSpring water treatment system's carbon-block filter effectively reduces more than 140 contaminants that can potentially affect your health.



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Porous Media

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Waterborne Contaminants

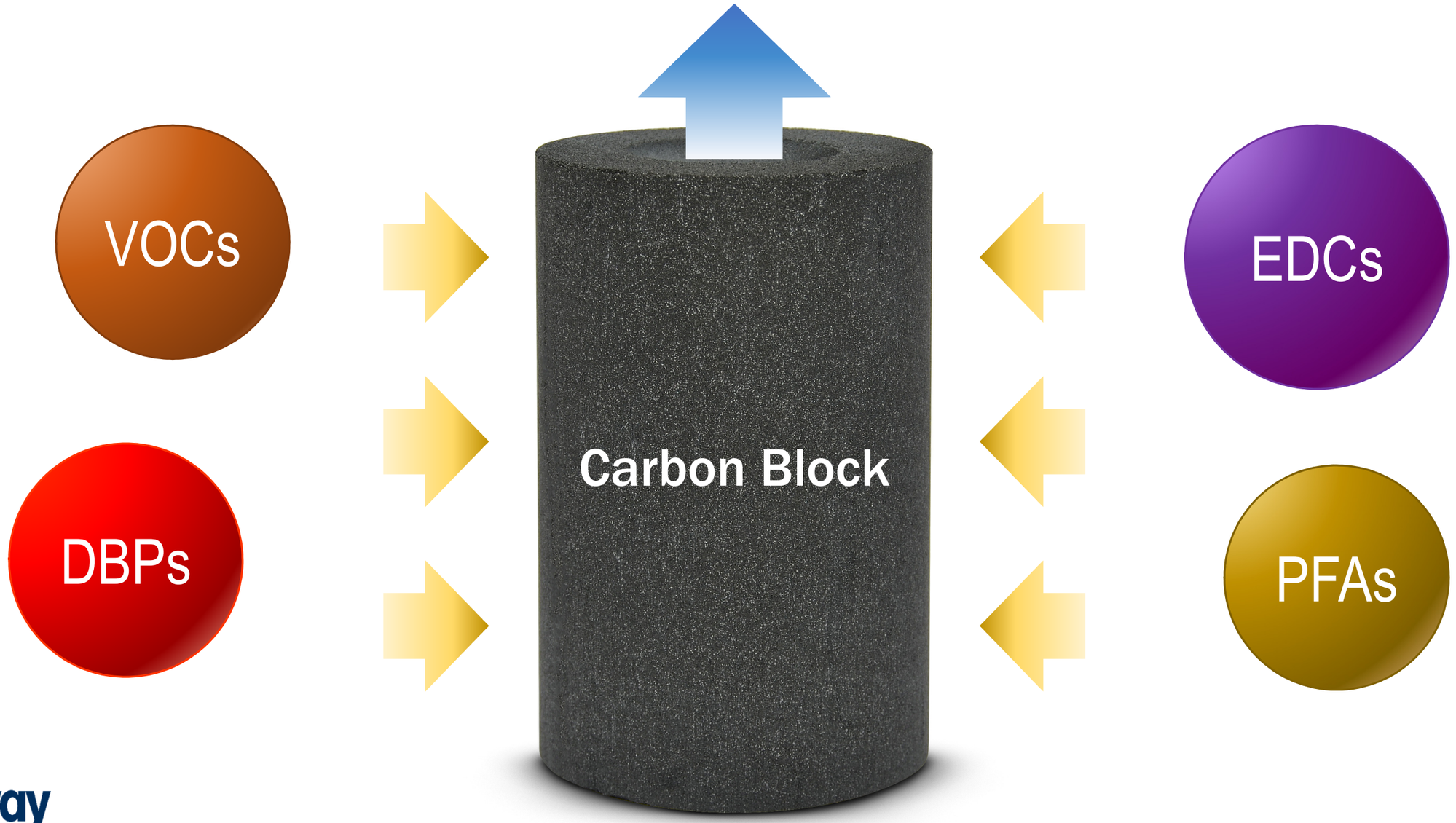

Figure 1. *Activated carbon block and contaminants in water.*

Mass Transfer in Porous Media

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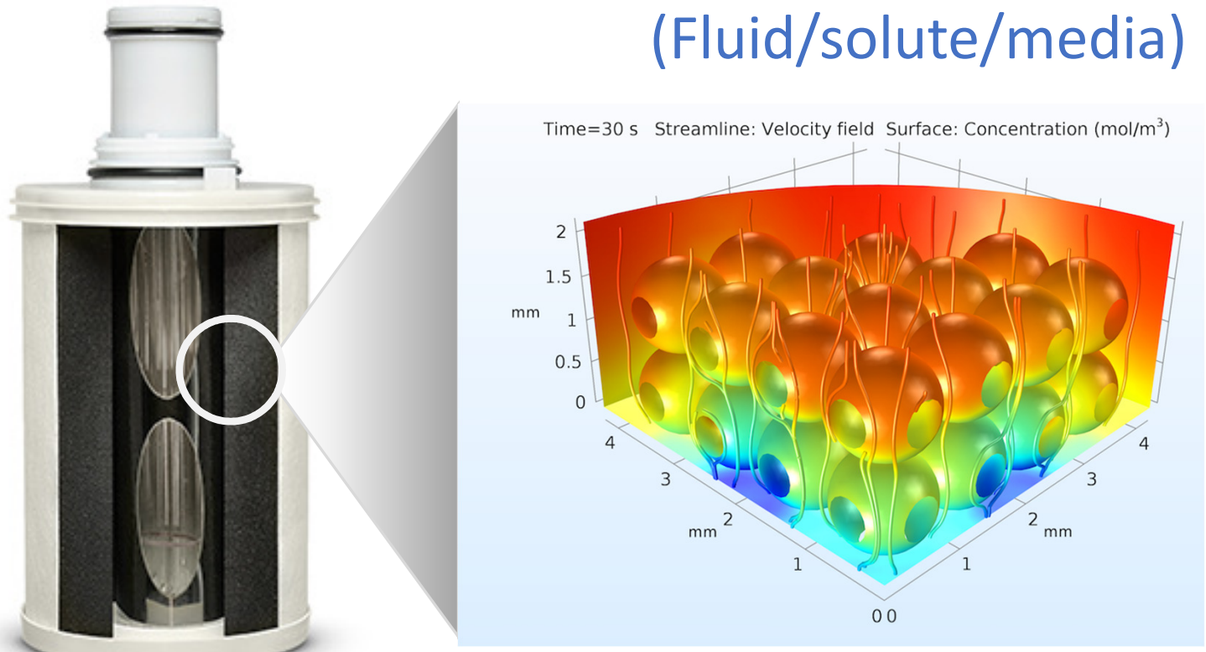
- Characteristics
  - Flow direction: outside-in radial
  - Dynamic working pressure: 60 psi
  - Flow rate: 0.9 gpm
  - Contact time: < 1 min
  - Reynolds number
    $Re = \frac{UL}{\nu}$ = ~2,100, laminar flow
  - Peclet number
    $Pe = \frac{UL}{D}$ >> 1, advection dominant
  - Permeability
    k = 10^{-9} to 10^{-10} m^2



Reference: Dickinson, 2017, COMSOL Blog

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RSSCT vs. COMSOL

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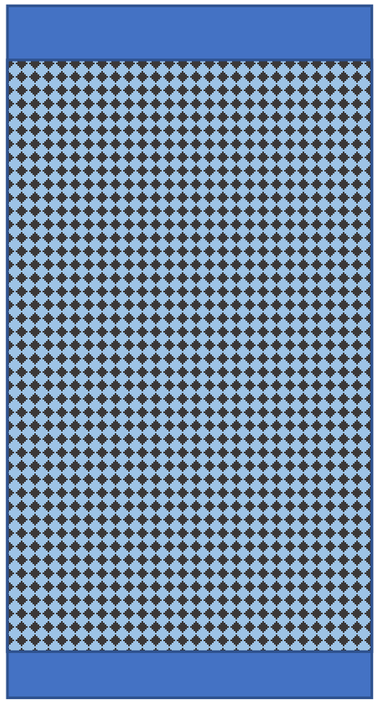
- Rapid Small-scale Column Test (RSSCT) models
  - constant pattern homogeneous surface diffusion model (CPHSDM)
  - pore surface diffusion model (PSDM)
  - Widely used from 1990's
  - Two-dimensional
  - Assumes ideal one-directional plug-flow system
  - Homogeneous media
  - Best for slow-flow packed bed reactors

- COMSOL Multiphysics®
  - Three-dimensional/2-D Axisymmetric
  - Calculate complex flow patterns
  - Enables heterogeneous media study
  - Ability to model various structural designs
  - Simultaneously calculates mass balance in the porous media/fluid regime



RSSCT

COMSOL Multyphysics®

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Process Diagram

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- Import Geometry (CAD STEP)
- Structural Analysis
- Geometry Builder
- Unify structure (Booleans and Partitions)
- Define boundary conditions
- Define materials
- Define inlet/outlets
- Define mesh

- Define dimensions (Q, r, d, L, A, u, etc.)
- Calculate characteristic parameters (Re, Pe, etc.)
- Determine flow regime (Laminar)
- Define fluid properties, wall conditions, initial fluid conditions
- Analyze flow pattern, ΔP, etc.

- Analyze flow/pressure
- Investigate flow patterns in pressure vessel
- Dynamic study of fluids/particles
- Particle Tracing Module
- Visualize movement of particles in the fluid in reactors.

- Calculate permeability
- Define porous media matrix
- Define diffusion coefficients
- Implement multi-physics study
- Analyze fluid movement in porous media
- Couple with reactor flow with porous media.

- Apply physical/chemical properties of media/solute
- Define mech./chem. reaction mechanism
- Analyze adsorption kinetics, breakthrough of each solute
- Evaluate heat effect on chemical reaction.
- Optimize product design.

***Figure 3**. Process diagram.*

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Model Equations

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- Mass transport equation (convection-diffusion)

$$\frac{\partial\left(\varepsilon_p c_A + \rho c_{p,A}\right)}{\partial t} + \nabla \cdot \left(-D_{e,A}\nabla c_A\right) + u \cdot \nabla c_A = 0$$

where
ε_p and ρ is the porosity and the density (kg/m^3) of the porous media, respectively
c_A and $c_{p,A}$ is the aqueous and particle concentration of chemical species, A (mol/m^3)
u is the fluid velocity determined by the reactor design (m/s)
$D_{e,A}$ is the effective diffusivity of the chemical species, A (m^2/s)

- Adsorption isotherm (Langmuir)

$$c_{p,A} = \frac{c_{p,max,A} K_{L,A} c_A}{1 + K_{L,A} c_A}$$

where
- $c_{p,max,A}$ is the Langmuir adsorption maximum (mol/kg)
- $K_{L,A}$ is the Langmuir constant (m^3/mol)
- c_A is the aqueous concentration of chemical species, A (mol/m^3)

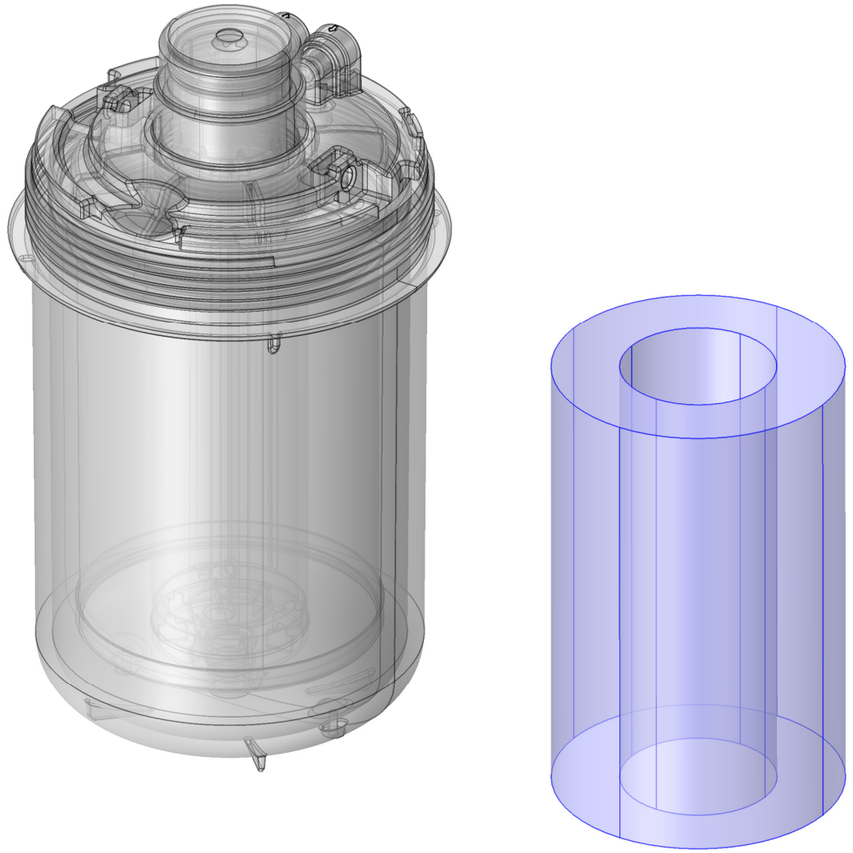

***Figure 2**. The three-dimensional carbon block geometry.*

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Model Equations

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Boundary Conditions

- Outlet pressure: $P = P_0 - \Delta P = 60$ psi (0.41 MPa)
- Inlet flow rate: $q_0 = 0.9$ gpm (3.41 L/min)
- Inflow concentration: $c = c_0$
- Wall conditions: no slip

Physics/Interface-selected

Fluid movement in the entire reactor:
Free and porous media flow (fp)

Mass transport of the chemical species in the porous media:
Transport of Diluted Species in Porous Media (tds)
interface with a time-dependent study step.

*contaminants level: ng/L (ppt) - μg/L (ppb)[17, 18]

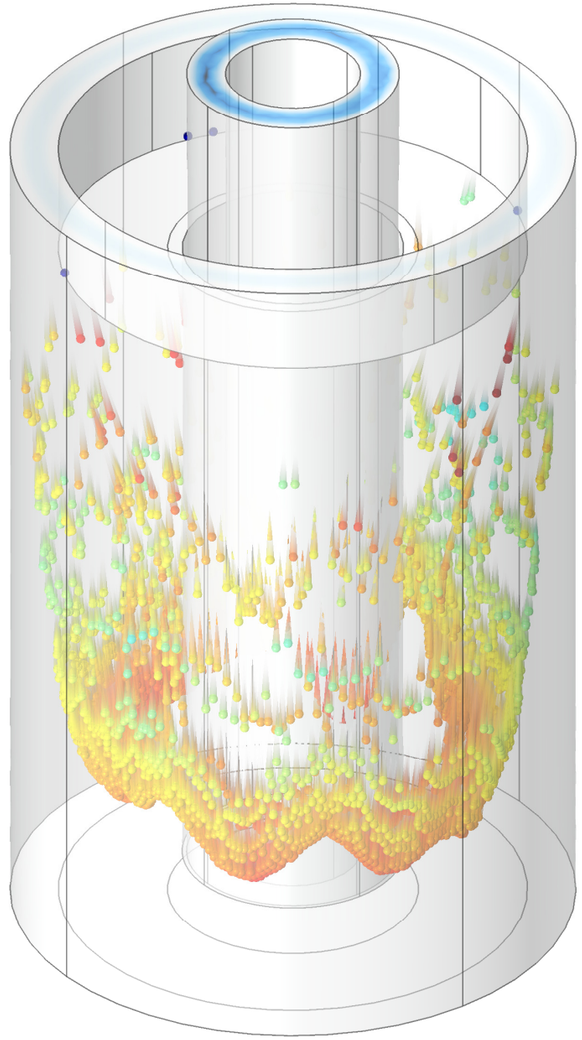

***Figure 2**. The three-dimensional carbon block geometry.*

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Test Conditions – Std. Method

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Test Protocol – NSF/ANSI 53

- NSF International Standard/American National Standard Institute
- Drinking Water Treatment Units (DTWUs) - Health Effect 53
- Influent concentration: ng/L (ppt) – ug/L (ppb)
  - Chloroform (VOC): 300 ppb
  - PFOA/PFOS: 1.5 ppb
  - Ibuprofen: 0.4 ppb

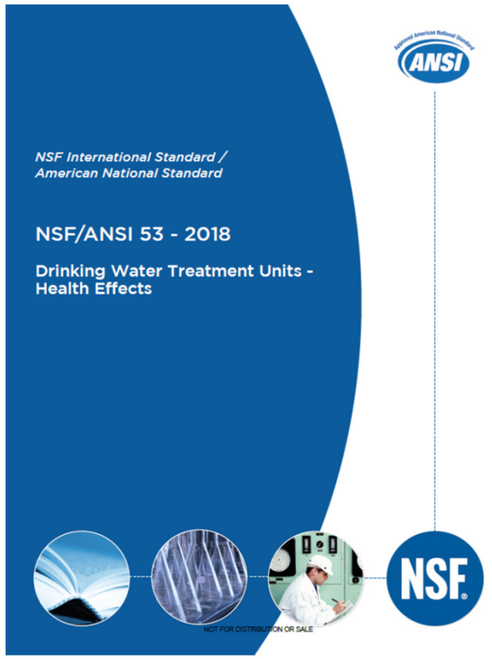

Table 7.1
Chemical reduction requirements

Substance	Individual influent sample point limits[1] (mg/L)	Average influent challenge[2] (mg/L)	Maximum effluent concentration (mg/L)	US EPA Method(s)[8,12]
ethylene dibromide	0.001 ± 50%	0.001 ± 10%	0.00005	504.1
heptachlor (H-34, heptox)	0.08 ± 40%	0.08 ± 10%	0.0004	505
heptachlor epoxide	0.004 ± 40%	0.004 ± 10%	0.0002	505
hexachlorocyclopentadiene	0.15 ± 40%	0.15 ± 10%	0.05	505
lindane	0.002 ± 40%	0.002 ± 10%	0.0002	505
methoxychlor[3]	0.12 ± 40%	0.12 ± 10%	0.04	505

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Full 3D vs. Axisymmetric

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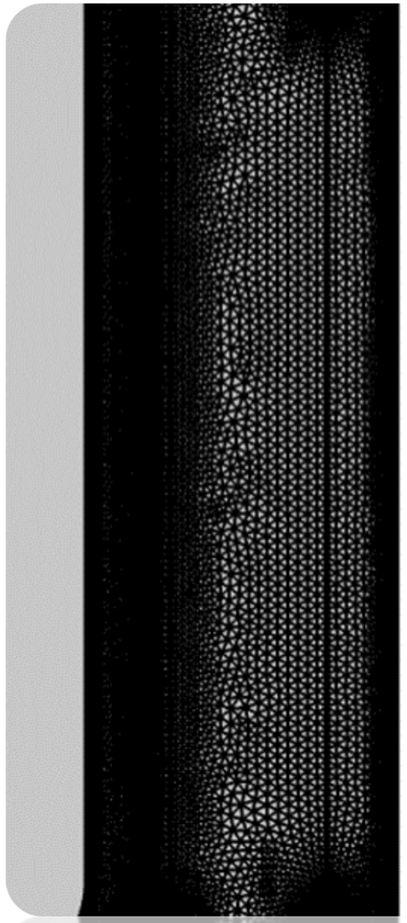
Computation time
~1 day



Computation time
~10 min

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***Figure 2**. Model component; (A) full three-dimensional and (B) Axisymmetrical mesh geometry.*

CFD Stationary Analysis

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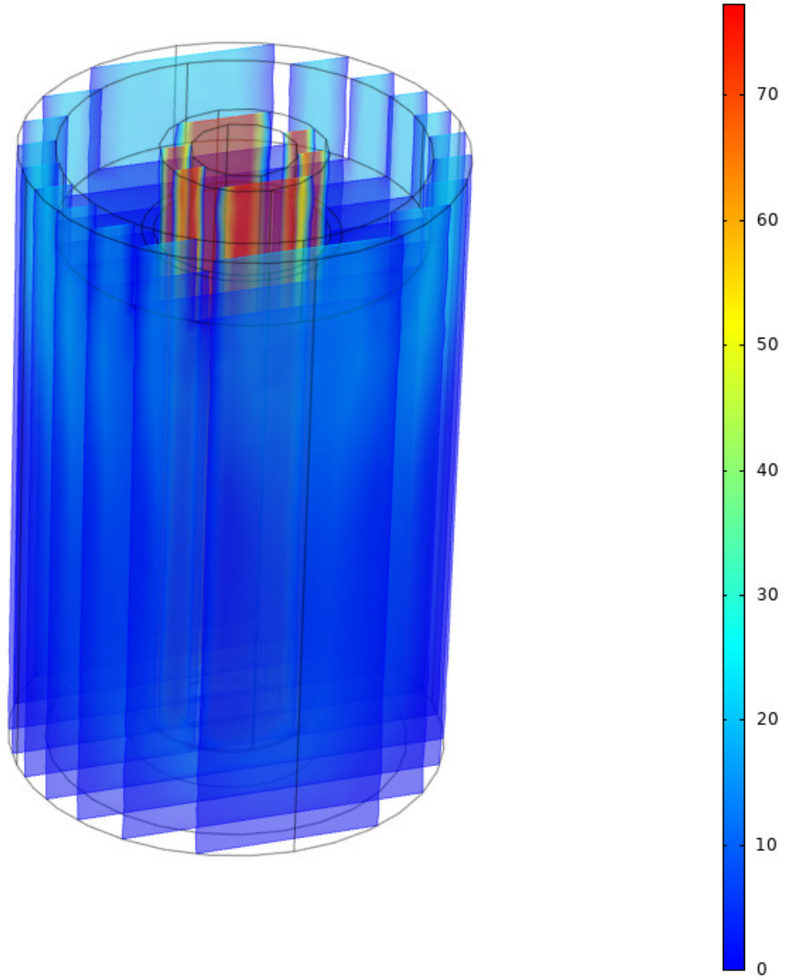
Flow



Pressure

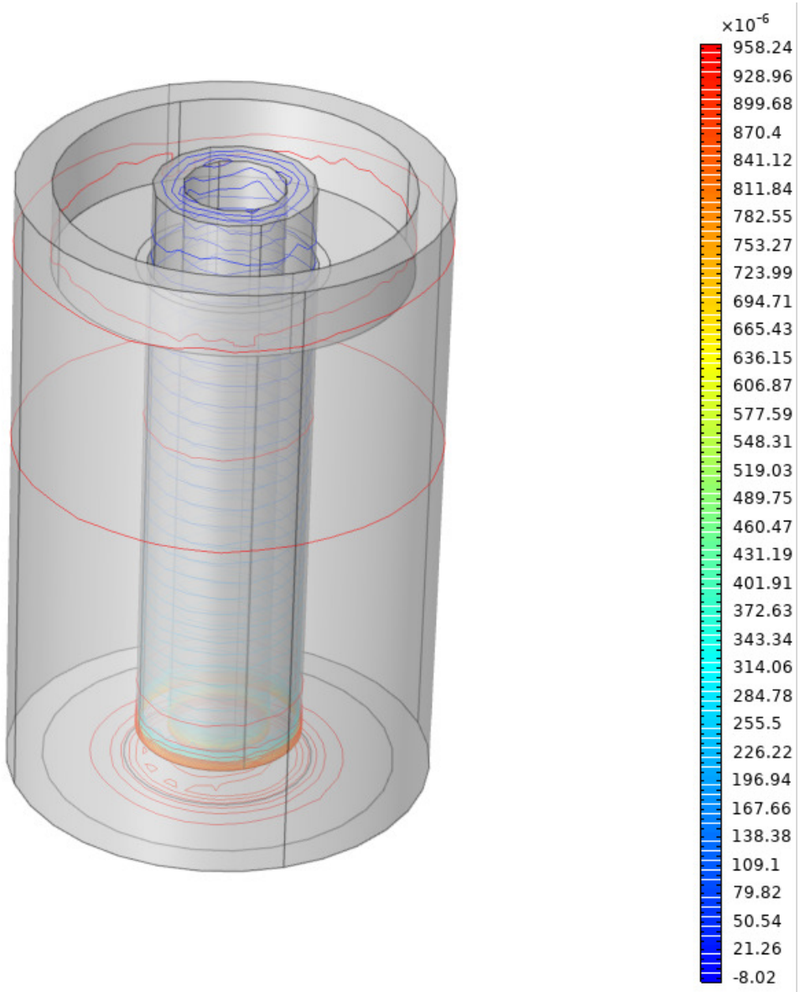


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***Figure 4**. Steady state flow analysis; (A) flow velocity (spf), (B) pressure (p).*

Time-dependent Analysis

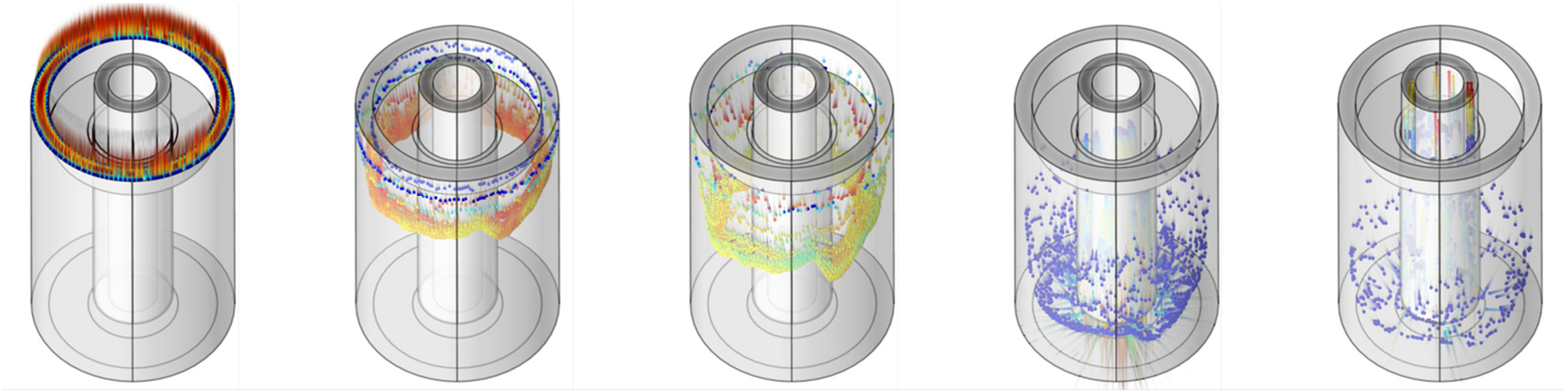
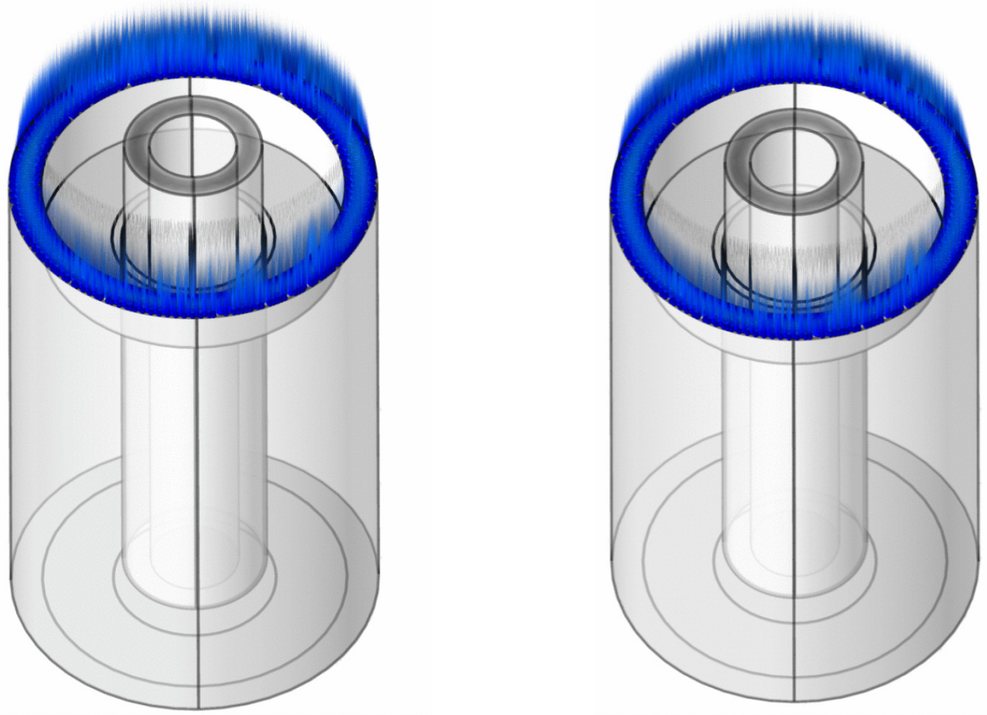


***Figure 5**. Time-dependent fluid dynamics analysis with Particle Tracing for Fluid Flow (fpt) physics interface.*



Animation (x4)

Chemical Adsorption Study

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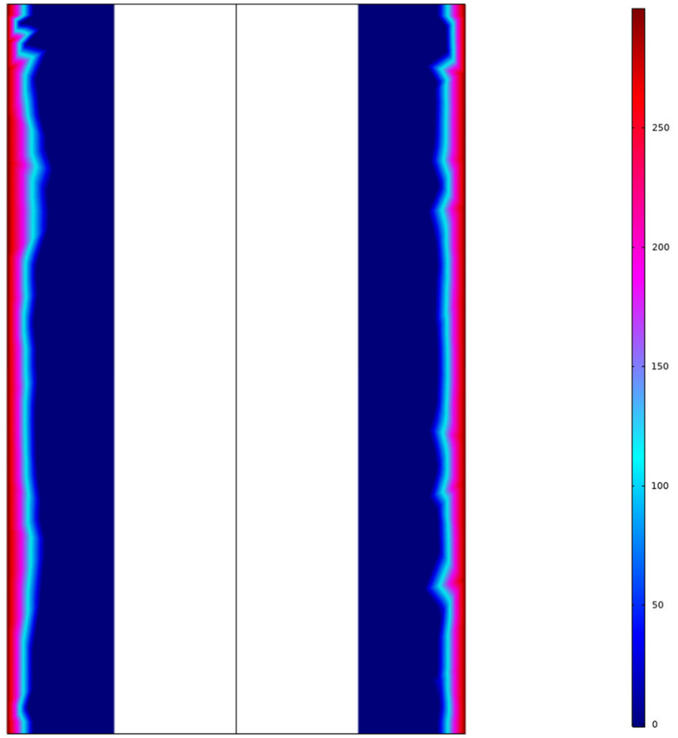
1. Organic simulations have been completed on 15 major species including 50 additional surrogated organic compounds (total 64 compounds).
2. Simulated for different influent concentration, flow rate, working pressure, temperature, reactor design, etc.



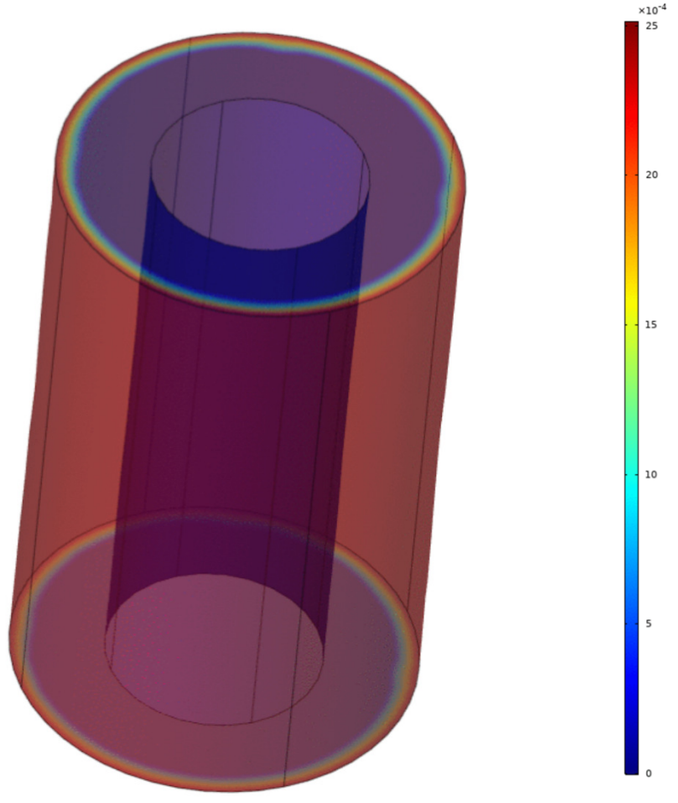


Figure 6. *Transport study (tds) of chemical species A, after 100 gallons volume treatment.*

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Chemical Adsorption Study

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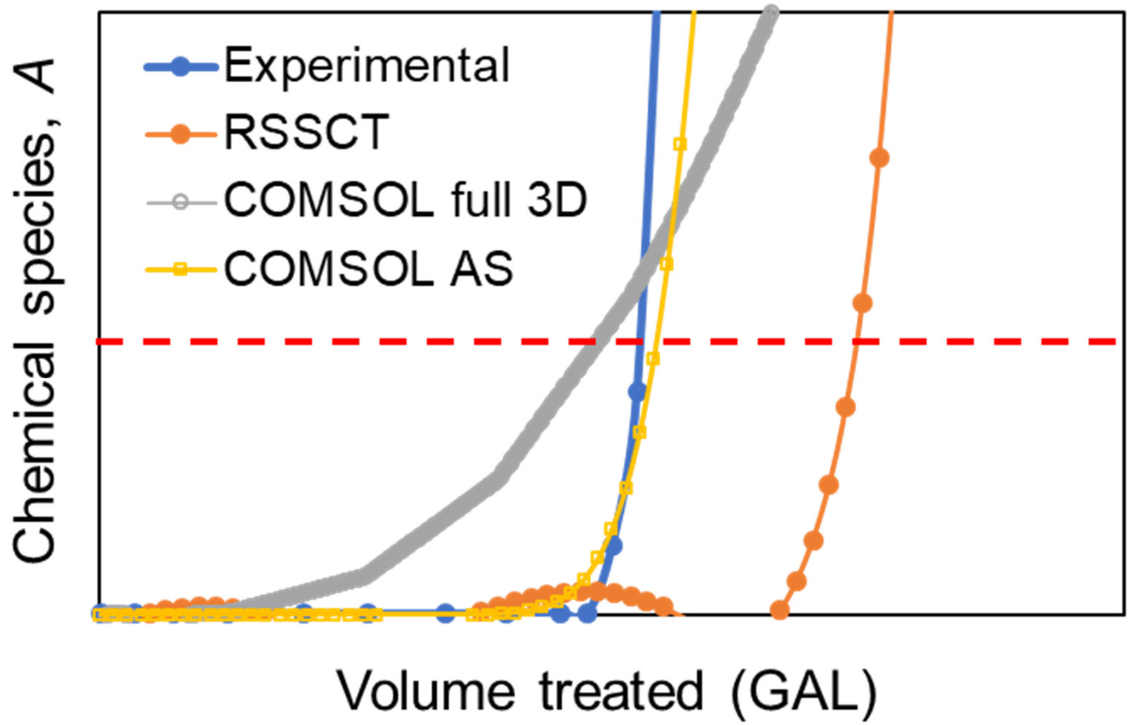

Model Name	Full 3D	AS
Predefined-mesh	Coarse	Finer
Number of Elements	14,852	16,854
Element quality	0.6741	0.9335
Volume/area ratio	0.1048	0.0362

	Error
Experimental	-
RSSCT-Packedbed 2D	+42.0%
COMSOL full 3D	-3.5%
COMSOL AS	+2.4%

Figure 7. *The averaged effluent concentration of species A from RSSCT and COMSOL simulations with respect to volume treated compared to the actual experimental result. The horizontal red dashed line: 5% breakthrough (95% reduction).*

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Chemical Adsorption Study

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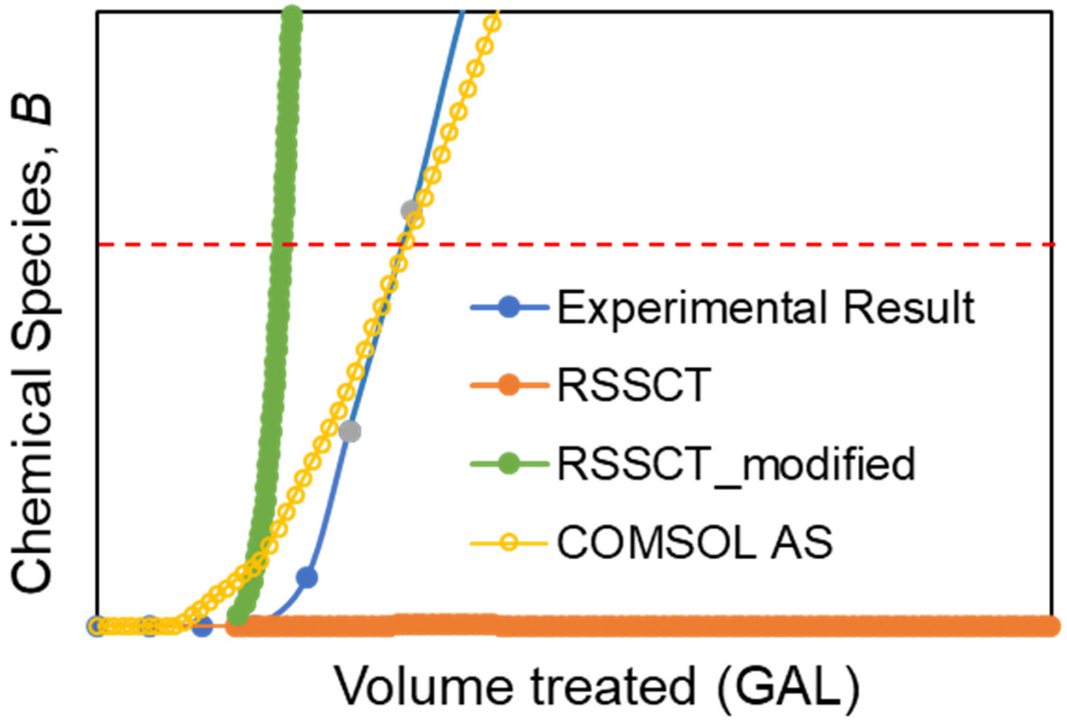

	Error
Experimental	-
RSSCT (Estimated Freundlich from Polanyi Isotherm Estimation)	+782.2%
RSSCT-modified (Experimental Freundlich)	-39.8%
COMSOL AS (Langmuir)	-0.9%

***Figure 8**. The averaged effluent concentration of species B from simulations with respect to volume treated compared to the actual experimental results. The red line: 5% breakthrough (95% reduction).*

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Conclusions

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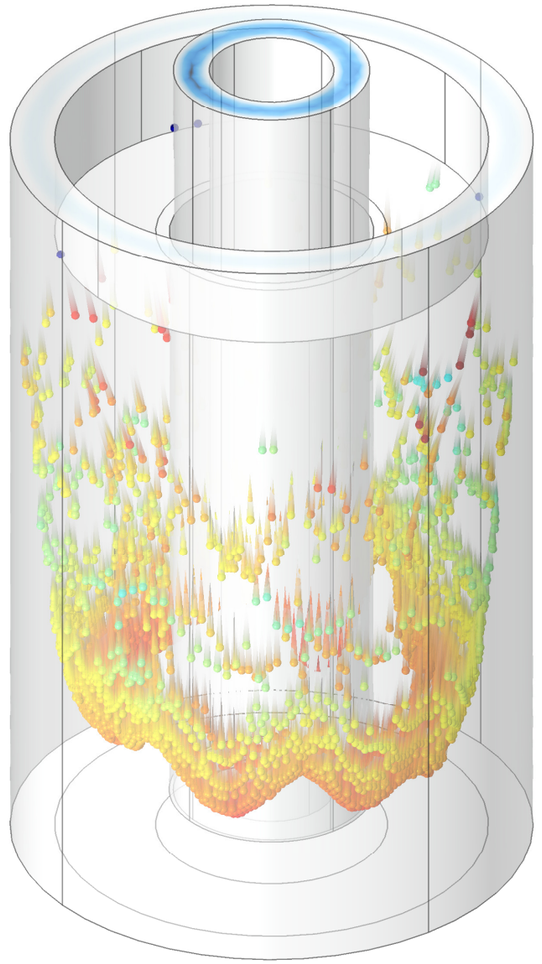
1. The COMSOL Multiphysics® model used in this transport and adsorption study successfully demonstrated not only **flow patterns** in the modulated reactor but also **chemical concentration changes** in the full-scale hollow cylindrical porous adsorbent structure.
2. To accurately simulate the adsorption phenomena in different reactors, both **adsorption isotherms** and **fluid movement** should be considered and compute simultaneously.
3. The results are critically important to enhance contaminant reduction performance by **optimizing design parameters** in similar reactor applications.
4. The transport/adsorption model can be used as a **platform** estimating the performance of other numerous chemical species and emerging contaminants which have different physical and chemical properties.



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Acknowledgement

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