



# Ceramic Water Filter with Activated Carbon Core

## *Introduction*

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This example illustrates how to model the transport of different contaminants through a ceramic water filter candle with an activated carbon core. This type of water filter can be found in tabletop gravity filters as well as attached to the faucet or as part of a larger reverse osmosis filter system. It shows how to set up the flow and transport equations to model different filter mechanisms and examines the effect of a small fracture in the ceramics part.

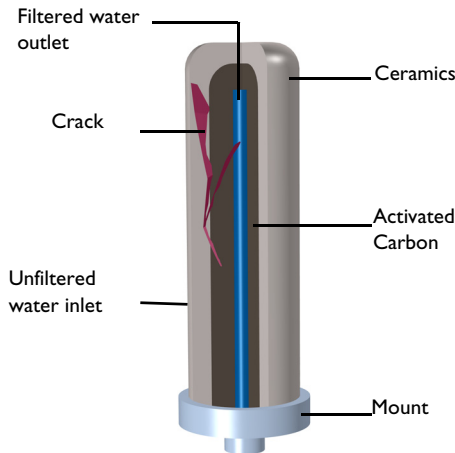
Our drinking water contains various impurities. These can be simply particles of dirt, which lead to turbidity of the water or cause unpleasant odors, such as chlorine. There can also be dangerous bacteria like *Escherichia coli*. That is why in many regions, water is disinfected by chlorination, thus destroying dangerous pathogens. The drawback of chlorination is on the one hand the resulting odor, on the other hand a reaction of chlorine with organic substances present in water can form harmful by-products such as the carcinogenic trihalomethanes.

Representative for these different pollutants, the model refers to chlorine and the trihalomethane chloroform. The term “particles” covers all substances that are filtered out of the water based solely on their size.

## *Model Definition*

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The model geometry is shown in [Figure 1](#). The geometric properties are listed in [Table 1](#).



*Figure 1: Sketch of the modeled filter.*

Tap water containing different impurities enters the filter with an inlet pressure of  $p_{in}=6$  psi. First, the water passes through the fine pored ceramic, in which particles with a larger diameter than the pore size are filtered out. The fracture in the ceramic has a relatively large aperture such that particles can travel almost unhindered and enter the activated carbon part.

TABLE 1: GEOMETRY PARAMETERS

Name	Value	Description
r_filter	2.2 cm	Filter radius
l_filter	14.5 cm	Filter length
th_ceramics	0.8 cm	Thickness ceramics
th_carbon	1 cm	Thickness carbon
th_attachement	4 mm	Thickness mount

Activated carbon has a large surface area and is mostly used in granular form in domestic water filters. The advantage of granular-activated carbon compared to powdered-activated carbon is the smaller pressure drop due to its relatively large particle size. At the same time this results in a smaller surface area available for reaction and adsorption. The effect on the adsorption capacity of trihalomethanes like chloroform is similar. The activated carbon is thus used up over time, which makes regular replacement of the filter necessary. In large filter systems the activated carbon can be backwashed.

### FLUID FLOW

The flow velocity  $\mathbf{u}$  (SI unit: m/s) through the filter depends on the gradient of the pressure  $p$  (SI unit: Pa) as described by Darcy's law.

$$\mathbf{u} = -\frac{\kappa}{\mu} \nabla p$$

Here,  $\kappa$  (SI unit:  $m^2$ ) and  $\mu$  (SI unit: Pa·s) are the permeability of the filter and dynamic viscosity of water, respectively. For the ceramic part a fixed value for the permeability is assumed and the permeability for the activated carbon is calculated according to the Kozeny–Carman equation.

$$\kappa = \frac{d_p^2}{180} \frac{\epsilon_p^3}{(1 - \epsilon_p)^2}$$

The flow in the fracture is in general much faster than in the surrounding porous matrix. The cubic law is a common correlation for modeling fracture flow. It defines the permeability  $\kappa_f$  (SI unit:  $m^2$ ) in the fracture according to

$$\kappa_f = \frac{d_f^2}{12f_f}$$

The values used to set up Darcy's law for the different sections are listed in [Table 2](#).

TABLE 2: DARCY'S LAW PARAMETER

Name	Value	Description
por_ceramics	0.18	Porosity, ceramics
por_carbon	0.45	Porosity, activated carbon
por_fracture	0.7	Porosity fracture
df	0.2 mm	Fracture aperture
dp_carbon	20 $\mu\text{m}$	Granular carbon diameter
kappa_ceramics	$8 \cdot 10^{-12} \text{ m}^2$	Permeability ceramics
p_in	6 psi	Inlet pressure

### CONTAMINANT TRANSPORT

Precise values of reaction of chlorine and adsorption rates of chloroform must be measured for each type of activated carbon. Adsorption is modeled using a Freundlich adsorption isotherm. The values used in this model are listed in the [Table 3](#).

TABLE 3: TRANSPORT PROPERTIES

Name	Value	Description
R_cl	0.39 l/s	Reaction rate chlorine
S_cp	-0.16 l/s	Particle sink term
Kf	10	Freundlich constant, chloroform
Nf	2	Freundlich exponent, chloroform
cref_chcl3	$0.5 \text{ mol/m}^3$	Reference concentration, chloroform

The simulation covers a period of two minutes. Afterward, a quasi-stationary state is reached and the filter efficiency can be determined.

## Results and Discussion

The pressure and velocity field is shown in [Figure 2](#).

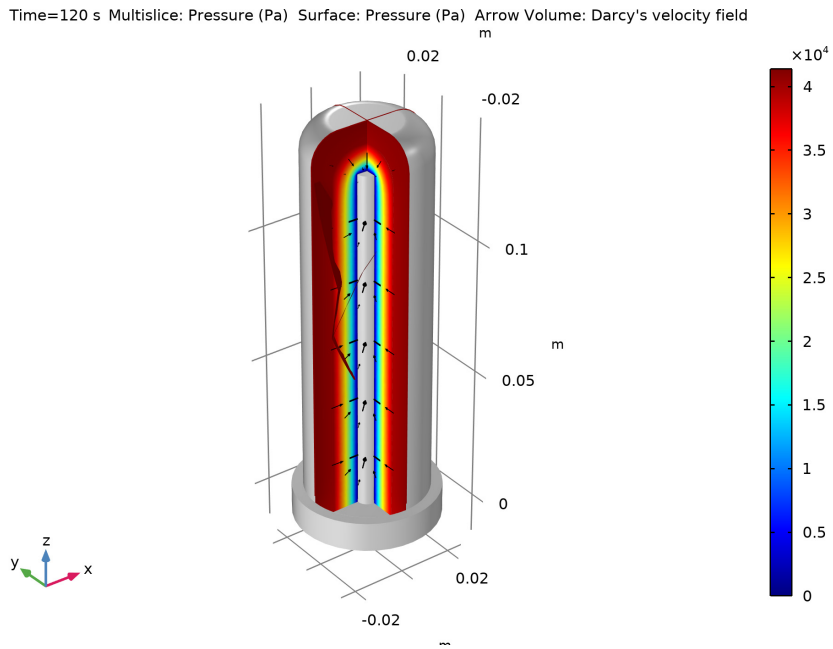
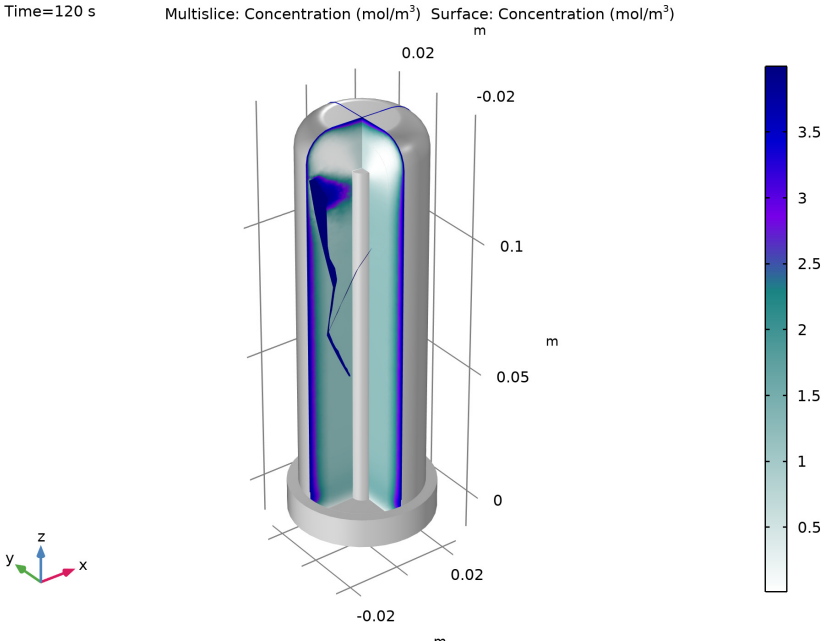


Figure 2: Pressure distribution (color) and flow field (arrows).

The particle concentration after 2 minutes is shown in [Figure 3](#). One can see that the particles are filtered out immediately at the surface. It is mainly the fracture that allows the particles to pass the filter.



*Figure 3: Particle concentration in the filter.*

Figure 4 shows the chlorine concentration after 2 minutes. After chlorine has passed the ceramic part, it is removed from the water by the reaction with activated carbon.

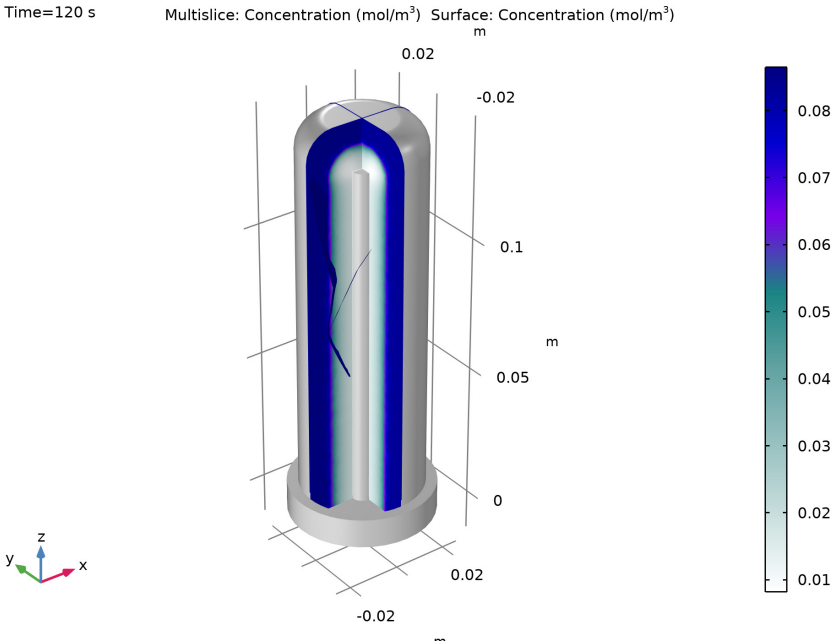
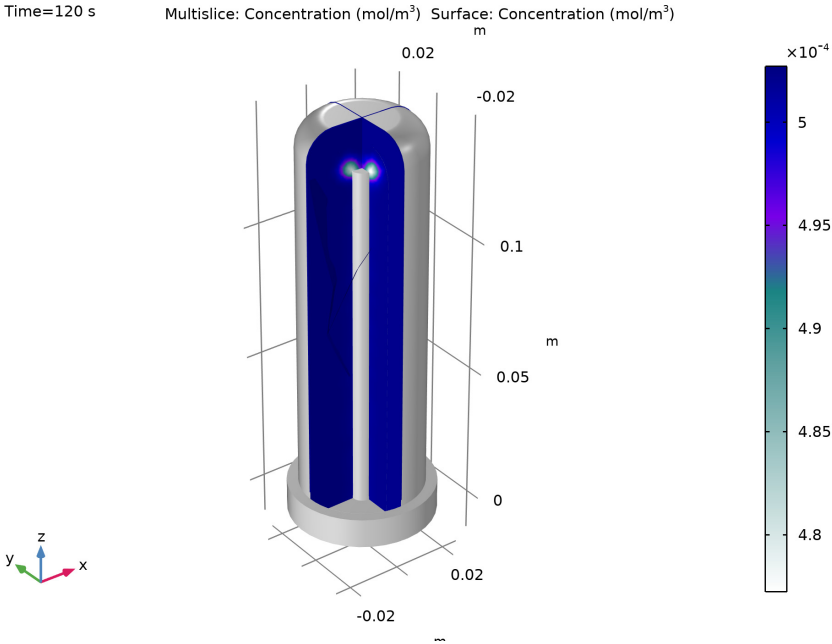


Figure 4: Chlorine concentration after 2 minutes.

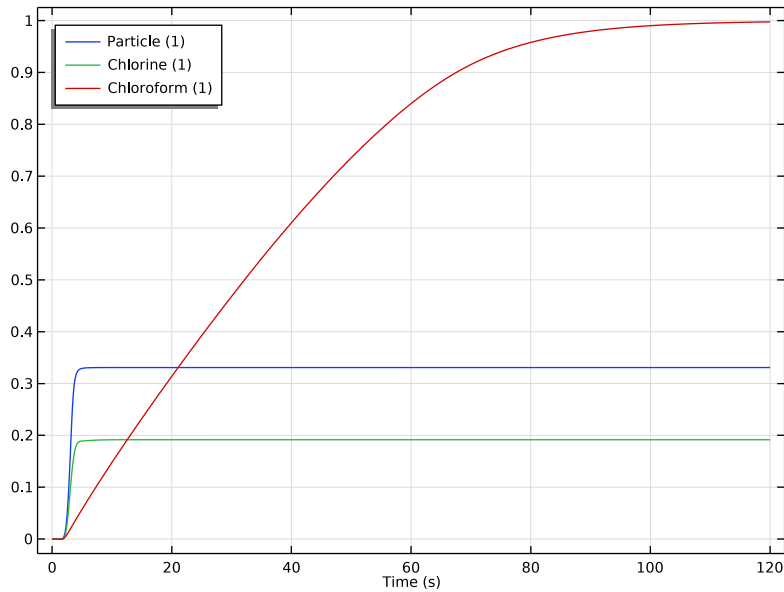
The concentration of dangerous chloroform is shown in [Figure 5](#). It clearly shows that this filter is not suitable for the removal of chloroform. Usually, trihalomethanes are already filtered in the waterworks, with a very strict upper limit — often 0.



*Figure 5: Chloroform concentration after 2 minutes.*



To evaluate the performance of this filter, we evaluate the ratio between the concentration at the outlet and the concentration at the inlet as shown in [Figure 6](#).



*Figure 6: Effectiveness of the filter. Ratio of the concentration at the outlet to the initial concentration.*

### *Notes About the COMSOL Implementation*

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In this model it is assumed that the flow field does not depend on the species concentrations. This is a reasonable assumption for the time interval considered. If the filter is examined over a long period of time, the particles clog the pores of the ceramic, which leads to a higher pressure drop. In addition, the activated carbon is used up, which means that less chlorine and chloroform is removed.

The fracture in the ceramic filter is implemented as a surface within the 3D domain. This is possible due to the special boundary conditions that are available for the Darcy's Law and the Transport of Diluted Species interface. They make it possible to simplify the model geometry to save computational resources.

### *Reference*

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1. <https://www.freshwatersystems.com/blogs/blog>

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**Application Library path:** Porous\_Media\_Flow\_Module/Solute\_Transport/  
ceramic\_water\_filter

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### *Modeling Instructions*

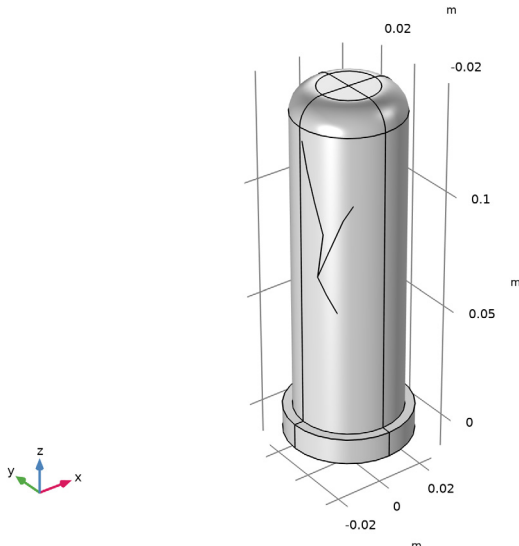
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#### **ROOT**

Start by opening a file that already contains the geometry sequence as well as selections that are used for setting up the physics. The file also contains all important parameters, divided into three parameter lists for a better overview.

- 1 From the **File** menu, choose **Open**.
- 2 Browse to the model's Application Libraries folder and double-click the file ceramic\_water\_filter\_geom\_sequence.mph.



#### **GEOMETRY 1**



#### **MATERIALS**

Continue with adding the materials. Water is used from the built-in material library. All other materials are user defined.

## ADD MATERIAL

- 1 In the **Home** toolbar, click  **Add Material** to open the **Add Material** window.
- 2 Go to the **Add Material** window.
- 3 In the tree, select **Built-in>Water, liquid**.
- 4 Click **Add to Component** in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## MATERIALS

### *Ceramics*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, type Ceramics in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Ceramics**.

### *Activated carbon*


- 1 Right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, type Activated carbon in the **Label** text field.
- 3 Locate the **Geometric Entity Selection** section. From the **Selection** list, choose **Carbon**.

### *Fracture*

- 1 Right-click **Materials** and choose **Blank Material**.
- 2 In the **Settings** window for **Material**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 From the **Selection** list, choose **Fracture**.
- 5 In the **Label** text field, type Fracture.

Which material properties are required will be determined during the physics setup. Continue with defining the Darcy's Law and Transport of Diluted Species in Porous Media interfaces.

## ADD PHYSICS

- 1 In the **Home** toolbar, click  **Add Physics** to open the **Add Physics** window.
- 2 Go to the **Add Physics** window.
- 3 In the tree, select **Fluid Flow>Porous Media and Subsurface Flow>Darcy's Law (dl)**.
- 4 Click **Add to Component 1** in the window toolbar.

5 In the tree, select **Chemical Species Transport**>  
**Transport of Diluted Species in Porous Media (tds)**.

6 Click **Add to Component 1** in the window toolbar.

The geometry also contains the mount, which is not relevant for the simulation. Each interface should be active on the modeling domains only.

### **DARCY'S LAW (DL)**

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Darcy's Law (dl)**.

2 In the **Settings** window for **Darcy's Law**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Modeling domains**.

### *Fluid and Matrix Properties 1*

1 In the **Model Builder** window, under **Component 1 (comp1)**>**Darcy's Law (dl)** click **Fluid and Matrix Properties 1**.

2 In the **Settings** window for **Fluid and Matrix Properties**, locate the **Fluid Properties** section.

3 From the **Fluid material** list, choose **Water, liquid (mat1)**.

4 Locate the **Matrix Properties** section. From the **Porous material** list, choose **Ceramics (mat2)**.

### *Fluid and Matrix Properties 2*

1 In the **Physics** toolbar, click  **Domains** and choose **Fluid and Matrix Properties**.

2 In the **Settings** window for **Fluid and Matrix Properties**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Carbon**.

4 Locate the **Fluid Properties** section. From the **Fluid material** list, choose **Water, liquid (mat1)**.

5 Locate the **Matrix Properties** section. From the **Permeability model** list, choose **Kozeny-Carman**.

6 In the  $d_p$  text field, type dp\_carbon.

### *Fracture Flow 1*

1 In the **Physics** toolbar, click  **Boundaries** and choose **Fracture Flow**.

2 In the **Settings** window for **Fracture Flow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Fracture**.

### *Fluid and Fracture Properties 1*


- 1 In the **Model Builder** window, expand the **Fracture Flow 1** node, then click **Fluid and Fracture Properties 1**.
- 2 In the **Settings** window for **Fluid and Fracture Properties**, locate the **Fluid Properties** section.
- 3 From the **Fluid material** list, choose **Water, liquid (mat1)**.
- 4 Locate the **Fracture Properties** section. From the **Porous material** list, choose **Fracture (mat4)**.
- 5 From the **Permeability model** list, choose **Cubic law**.

### *Aperture 1*


- 1 In the **Model Builder** window, click **Aperture 1**.
- 2 In the **Settings** window for **Aperture**, locate the **Aperture** section.
- 3 In the  $d_f$  text field, type  $df$ .

### *Pressure 1*

A pressure of 6psi is assumed as inlet condition. This is a typical value for the pressure acting on a filter connected to the water supply.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Pressure**.
- 2 In the **Settings** window for **Pressure**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Unfiltered water inlet**.
- 4 Locate the **Pressure** section. In the  $p_0$  text field, type  $p\_in$ .

### *Pressure 2*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Pressure**.
- 2 In the **Settings** window for **Pressure**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Filtered water outlet**.

## **TRANSPORT OF DILUTED SPECIES IN POROUS MEDIA (TDS)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Transport of Diluted Species in Porous Media (tds)**.

The transport of three different substances is studied: particles which are filtered in the ceramic due to their size, chlorine which reacts with the activated carbon, and chloroform which is adsorbed by the activated carbon.

- 2 In the **Settings** window for **Transport of Diluted Species in Porous Media**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Modeling domains**.

Add the corresponding variables for the different compounds.

4 Click to expand the **Dependent Variables** section. In the **Number of species** text field, type 3.

5 In the **Concentrations** table, enter the following settings:

c_p
c_c1
c_chcl3

#### *Fluid 1*

1 In the **Model Builder** window, under **Component 1 (comp1)>**

**Transport of Diluted Species in Porous Media (tds)>Porous Medium 1** click **Fluid 1**.

2 In the **Settings** window for **Fluid**, locate the **Convection** section.

3 From the **u** list, choose **Darcy's velocity field (dl)**.

Duplicate this node and define the adsorption properties of chloroform on activated carbon.

#### *Porous Medium 2*

1 In the **Model Builder** window, under **Component 1 (comp1)>**

**Transport of Diluted Species in Porous Media (tds)** right-click **Porous Medium 1** and choose **Duplicate**.

2 In the **Settings** window for **Porous Medium**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Carbon**.

#### *Adsorption 1*

1 In the **Physics** toolbar, click  **Attributes** and choose **Adsorption**.

2 In the **Settings** window for **Adsorption**, locate the **Adsorption** section.

3 From the **Adsorption isotherm** list, choose **Freundlich**.

4 Select the **Species c\_chcl3** check box.


5 In the  $K_{F,cchcl3}$  text field, type Kf.

6 In the  $N_{F,cchcl3}$  text field, type Nf.

7 In the  $c_{ref,cchcl3}$  text field, type cref\_chcl3.


#### *Species Source 1*

The filtration of the particles can be described as a sink term. In contrast, chlorine and chloroform are not removed.


- 1 In the **Physics** toolbar, click  **Domains** and choose **Species Source**.
- 2 In the **Settings** window for **Species Source**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Ceramics**.
- 4 Locate the **Species Source** section. In the  $S_{cp}$  text field, type  $S_{cp}*c_p$ .

#### *Reactions I*

Chlorine is removed from the water by a reaction with carbon.


- 1 In the **Physics** toolbar, click  **Domains** and choose **Reactions**.
- 2 In the **Settings** window for **Reactions**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Carbon**.
- 4 Locate the **Reaction Rates** section. In the  $R_{ccl}$  text field, type  $-R_{c1}*c_{c1}$ .

#### *Fracture I*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Fracture**.
- 2 In the **Settings** window for **Fracture**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Fracture**.
- 4 Locate the **Fracture Properties** section. In the  $d_{fr}$  text field, type  $df$ .
- 5 Locate the **Convection** section. From the **u** list, choose **Darcy's velocity field (dl)**.
- 6 Locate the **Diffusion** section. From the **Fluid material** list, choose **Water, liquid (mat1)**.

#### *Concentration I*

To complete the physics setup add the boundary conditions for the transport equations.

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Concentration**.
- 2 In the **Settings** window for **Concentration**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Unfiltered water inlet**.
- 4 Locate the **Concentration** section. Select the **Species c\_p** check box.
- 5 In the  $c_{0,cp}$  text field, type  $c_{p0}$ .
- 6 Select the **Species c\_cl** check box.
- 7 In the  $c_{0,ccl}$  text field, type  $c_{c10}$ .
- 8 Select the **Species c\_chcl3** check box.
- 9 In the  $c_{0,cchcl3}$  text field, type  $c_{chc130}$ .

#### *Outflow I*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outflow**.
- 2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.

3 From the **Selection** list, choose **Filtered water outlet**.

Now the missing material properties can be added.

## MATERIALS

### *Ceramics (mat2)*

1 In the **Model Builder** window, under **Component 1 (comp1)**>**Materials** click **Ceramics (mat2)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Porosity	epsilon	por_ceramics	l	Basic
Permeability	kappa_iso ; kappaij = kappa_iso, kappaij = 0	kappa_ceramics	m <sup>2</sup>	Basic

### *Activated carbon (mat3)*

1 In the **Model Builder** window, click **Activated carbon (mat3)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Porosity	epsilon	por_carbon	l	Basic
Density	rho	375 [kg/m <sup>3</sup> ]	kg/m <sup>3</sup>	Basic

### *Fracture (mat4)*

1 In the **Model Builder** window, click **Fracture (mat4)**.

2 In the **Settings** window for **Material**, locate the **Material Contents** section.

3 In the table, enter the following settings:


Property	Variable	Value	Unit	Property group
Porosity	epsilon	por_fracture	l	Basic



## MESH 1

Set up a proper mesh. High gradients for the particle concentration are expected at the filter boundaries due to the relatively large sink term. These gradients can be efficiently resolved with a boundary layer mesh. Also limit the maximum element size to resolve the geometry properly.


### *Free Triangular 1*

- 1 In the **Mesh** toolbar, click  **Boundary** and choose **Free Triangular**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Fracture**.

### *Size 1*

- 1 Right-click **Free Triangular 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.
- 5 In the associated text field, type 0.001.


### *Free Tetrahedral 1*

- 1 In the **Mesh** toolbar, click  **Free Tetrahedral**.
- 2 In the **Settings** window for **Free Tetrahedral**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Modeling domains**.

### *Size 1*

- 1 Right-click **Free Tetrahedral 1** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Extra fine**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section. Select the **Maximum element size** check box.
- 6 In the associated text field, type `th_ceramics/3`.

### *Boundary Layers 1*

- 1 In the **Mesh** toolbar, click  **Boundary Layers**.
- 2 In the **Settings** window for **Boundary Layers**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 From the **Selection** list, choose **Ceramics**.


### *Boundary Layer Properties*

- 1 In the **Model Builder** window, click **Boundary Layer Properties**.
- 2 In the **Settings** window for **Boundary Layer Properties**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Unfiltered water inlet**.
- 4 Locate the **Boundary Layer Properties** section. In the **Number of boundary layers** text field, type 5.

### *Free Tetrahedral 2*


In the **Mesh** toolbar, click  **Free Tetrahedral**.

### *Size*

- 1 In the **Model Builder** window, click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Extra fine**.
- 4 Click  **Build All**.

## **ADD STUDY**

The simulation should cover 2 minutes. Within this time interval the flow can be regarded as independent of the concentration.

- 1 In the **Home** toolbar, click  **Add Study** to open the **Add Study** window.
- 2 Go to the **Add Study** window.
- 3 Find the **Studies** subsection. In the **Select Study** tree, select **General Studies>Stationary**.
- 4 Find the **Physics interfaces in study** subsection. In the table, clear the **Solve** check box for **Transport of Diluted Species in Porous Media (tds)**.
- 5 Click **Add Study** in the window toolbar.


## **STUDY I**

- 1 In the **Model Builder** window, click **Study I**.
- 2 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 3 Clear the **Generate default plots** check box.



### *Step 1: Stationary*

Solve the stationary Darcian flow field, followed by a transient study step for the species transport.

### *Time Dependent*

- 1 In the **Study** toolbar, click  **Study Steps** and choose **Time Dependent> Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.
- 3 In the table, clear the **Solve for** check box for **Darcy's Law (dl)**.
- 4 Locate the **Study Settings** section. In the **Output times** text field, type range (0, 0.1, 6) range (8, 2, 120).


### *Solution 1 (sol1)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.
- 3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 4 From the **Steps taken by solver** list, choose **Strict**.  
A tight time step, particularly at the beginning of the simulation, is necessary to resolve the transition from the initial values (zero concentrations) to the applied boundary conditions.
- 5 In the **Study** toolbar, click  **Compute**.

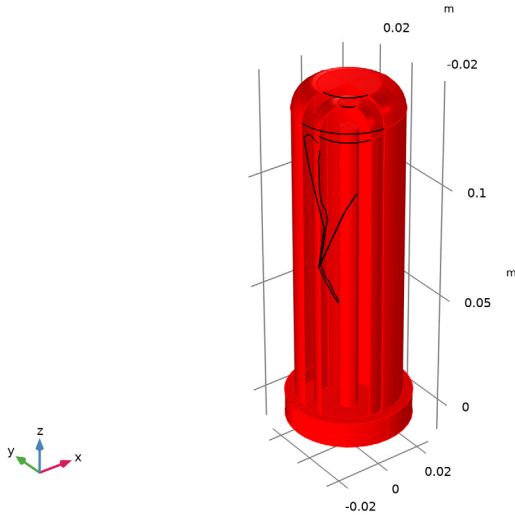
## **RESULTS**

Create a new dataset which is used to visualize the geometry.

### *Surface 1*


- 1 In the **Model Builder** window, expand the **Results** node.
- 2 Right-click **Results>Datasets** and choose **Surface**.
- 3 In the **Settings** window for **Surface**, locate the **Selection** section.
- 4 From the **Selection** list, choose **All boundaries**.
- 5 Click the  **Wireframe Rendering** button in the **Graphics** toolbar.

- 6 Press and hold the Ctrl key and mark the following boundaries in the **Selection** list: 11, 13, 15-18, 22, 24, and 36. Then click the **Remove from selection** button next to it.




To create [Figure 2](#), follow the steps below.

#### *Pressure*

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Pressure in the **Label** text field.
- 3 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

#### *Multislice 1*

- 1 In the **Pressure** toolbar, click  **More Plots** and choose **Multislice**.
- 2 In the **Settings** window for **Multislice**, locate the **Multipane Data** section.
- 3 Find the **Z-planes** subsection. In the **Planes** text field, type 0.

#### *Surface 1*

- 1 In the **Model Builder** window, right-click **Pressure** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, click to expand the **Inherit Style** section.
- 3 From the **Plot** list, choose **Multislice 1**.

#### *Selection 1*


- 1 Right-click **Surface 1** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.

3 From the **Selection** list, choose **Fracture**.


#### *Surface 2*

- 1 In the **Model Builder** window, right-click **Pressure** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Surface 1**.
- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 7 From the **Color** list, choose **Gray**.



#### *Arrow Volume 1*

- 1 Right-click **Pressure** and choose **Arrow Volume**.
- 2 In the **Settings** window for **Arrow Volume**, locate the **Coloring and Style** section.
- 3 From the **Color** list, choose **Black**.
- 4 In the **Pressure** toolbar, click  **Plot**.

#### *Particle concentration*

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Particle concentration in the **Label** text field.

#### *Multislice 1*

- 1 In the **Particle concentration** toolbar, click  **More Plots** and choose **Multislice**.
- 2 In the **Settings** window for **Multislice**, locate the **Expression** section.
- 3 In the **Expression** text field, type  $c_p$ .
- 4 Locate the **Multipane Data** section. Find the **Z-planes** subsection. In the **Planes** text field, type 0.
- 5 Locate the **Coloring and Style** section. From the **Color table** list, choose **AuroraAustralis**.
- 6 Click to expand the **Quality** section. From the **Recover** list, choose **Everywhere**.
- 7 In the **Particle concentration** toolbar, click  **Plot**.

Create the plot for the particle concentration as in [Figure 3](#).

#### *Surface 1*

- 1 In the **Model Builder** window, right-click **Particle concentration** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.

- 3 In the **Expression** text field, type `c_p`.
- 4 Locate the **Inherit Style** section. From the **Plot** list, choose **Multislice 1**.


#### *Selection 1*

- 1 Right-click **Surface 1** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Fracture**.

#### *Surface 2*

- 1 In the **Model Builder** window, right-click **Particle concentration** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Surface 1**.
- 4 Locate the **Expression** section. In the **Expression** text field, type `1`.
- 5 Locate the **Title** section. From the **Title type** list, choose **None**.
- 6 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 7 From the **Color** list, choose **Gray**.

#### *Particle concentration*

- 1 In the **Model Builder** window, click **Particle concentration**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Plot Settings** section.
- 3 Clear the **Plot dataset edges** check box.
- 4 In the **Particle concentration** toolbar, click  **Plot**.

#### *Chlorine concentration*

Duplicate this plot group to create the same plot for chlorine (Figure 4).

- 1 Right-click **Particle concentration** and choose **Duplicate**.
- 2 In the **Settings** window for **3D Plot Group**, type `Chlorine concentration` in the **Label** text field.

#### *Multislice 1*

- 1 In the **Model Builder** window, expand the **Chlorine concentration** node, then click **Multislice 1**.
- 2 In the **Settings** window for **Multislice**, locate the **Expression** section.
- 3 In the **Expression** text field, type `c_c1`.

#### *Surface 1*

- 1 In the **Model Builder** window, click **Surface 1**.

2 In the **Settings** window for **Surface**, locate the **Expression** section.

3 In the **Expression** text field, type `c_c1`.

4 In the **Chlorine concentration** toolbar, click  **Plot**.

Duplicate this plot again and repeat the steps to plot the chloroform concentration `c_chc13`. Compare with [Figure 5](#).

#### *Surface Average 1*

Finally, create [Figure 6](#).

1 In the **Results** toolbar, click  **More Derived Values** and choose **Average> Surface Average**.

2 In the **Settings** window for **Surface Average**, locate the **Selection** section.

3 From the **Selection** list, choose **Filtered water outlet**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
<code>c_p/c_p0</code>	1	Particle
<code>c_c1/c_c10</code>	1	Chlorine
<code>c_chc13/c_chc130</code>	1	Chloroform

5 Click  next to  **Evaluate**, then choose **New Table**.

#### **TABLE**

1 Go to the **Table** window.

2 Click **Table Graph** in the window toolbar.

#### **RESULTS**

##### *Table Graph 1*

1 In the **Model Builder** window, under **Results>ID Plot Group 5** click **Table Graph 1**.

2 In the **Settings** window for **Table Graph**, click to expand the **Legends** section.

3 Select the **Show legends** check box.

##### *Concentration over time.*

1 In the **Model Builder** window, under **Results** click **ID Plot Group 5**.

2 In the **Settings** window for **ID Plot Group**, type *Concentration over time*. in the **Label** text field.

3 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

