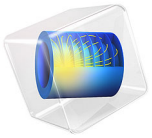


Ceramic Water Filter with Activated Carbon Core

Introduction

This example illustrates how to model the water flow and transport of different contaminants through a ceramic water filter candle with an activated carbon core and its housing. It shows how to set up the flow and transport equations to model different filter mechanisms and examines the effect of a 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

The model geometry is shown in Figure 1. The geometric properties are listed in Table 1.

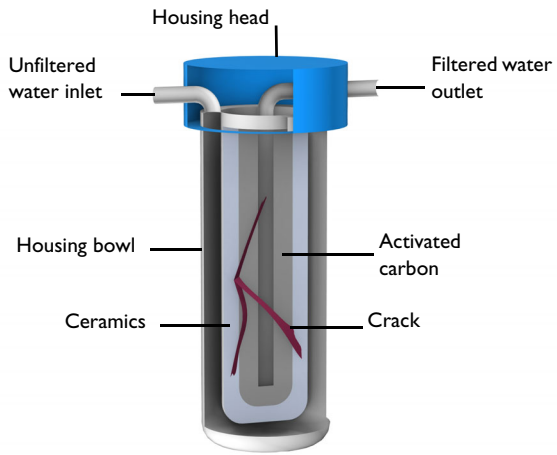


Figure 1: Sketch of the modeled filter.

Tap water containing different impurities enters the filter with a flow rate of approximately 2 l/min. First, the water flows into the housing bowl, then it passes through the fine pored

ceramic, in which particles with a larger diameter than the pore size are filtered out, and subsequently it flows through the activated carbon core into the outlet channel.

TABLE 1: GEOMETRY PARAMETERS

Name	Value	Description
r_filter	3.3 cm	Filter radius
l_filter	22 cm	Filter length
r_bowl	4.8 cm	Housing bowl radius
l_bowl	23.5 cm	Housing bowl length
r_head	6 cm	Housing head radius
h_head	4.5 cm	Housing head height
th_ceramics	1.2 cm	Thickness ceramics
th_carbon	1.5 cm	Thickness carbon

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 in the filter housing and the in- and outlet tubes is described by the Navier-Stokes equations:

$$\rho\frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} = \nabla\cdot[-p\mathbf{I} + \mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T)] + \mathbf{F}$$

$$\nabla\cdot\mathbf{u} = 0$$

In these equations, $\mathbf{u}$ denotes the velocity (SI unit: m/s), ρ the density (SI unit: kg/m^3), μ the dynamic viscosity (SI unit: Pa·s), and p the pressure (SI unit: Pa). The flow through the actual filter itself is described by Darcy's law:

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

Here, κ (SI unit: m^2) and μ (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.

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

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 κ_f (SI unit: m^2) in the fracture according to

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

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	200 μm	Granular carbon diameter
kappa_ceramics	$8 \cdot 10^{-12}$ m^2	Permeability ceramics

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	0.391/s	Reaction rate chlorine
S_cp	-0.16 1/s	Particle sink term
Kf	10	Freundlich constant, chloroform
Nf	2	Freundlich exponent, chloroform
cref_chcl3	0.5 mol/m^3	Reference concentration, chloroform

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

The pressure field is shown in Figure 2.

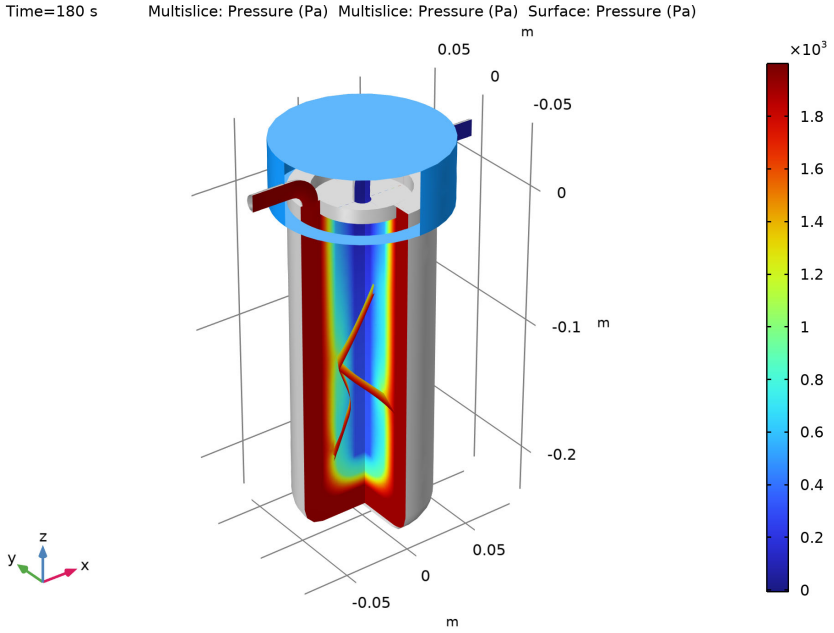


Figure 2: Pressure distribution.

The particle concentration after 3 minutes is shown in Figure 3. Observe that the particles are filtered out immediately at the surface. It is mainly the fracture that allows the particles to pass the filter.

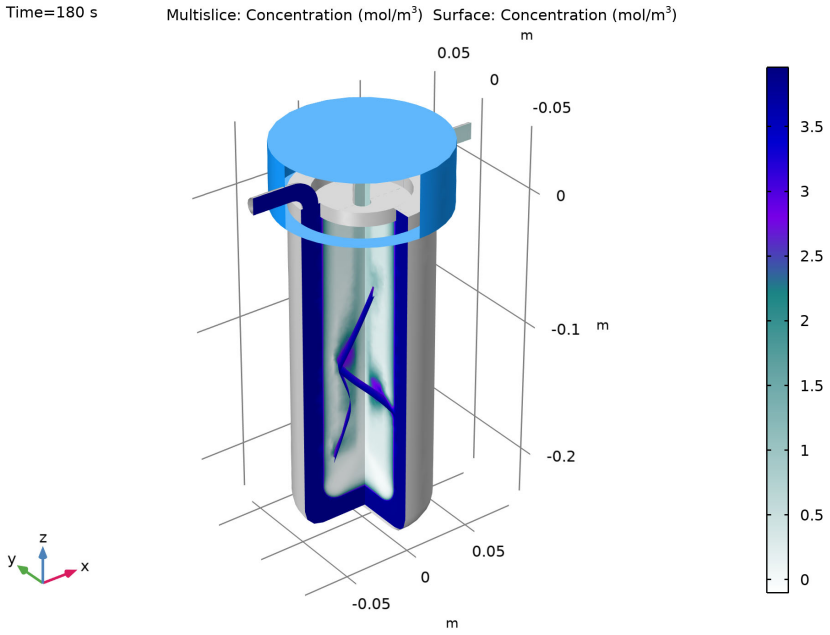


Figure 3: Particle concentration in the filter.

Figure 4 shows the chlorine concentration after 3 minutes. After chlorine has passed the ceramic part, it is removed from the water by the reaction with activated carbon.

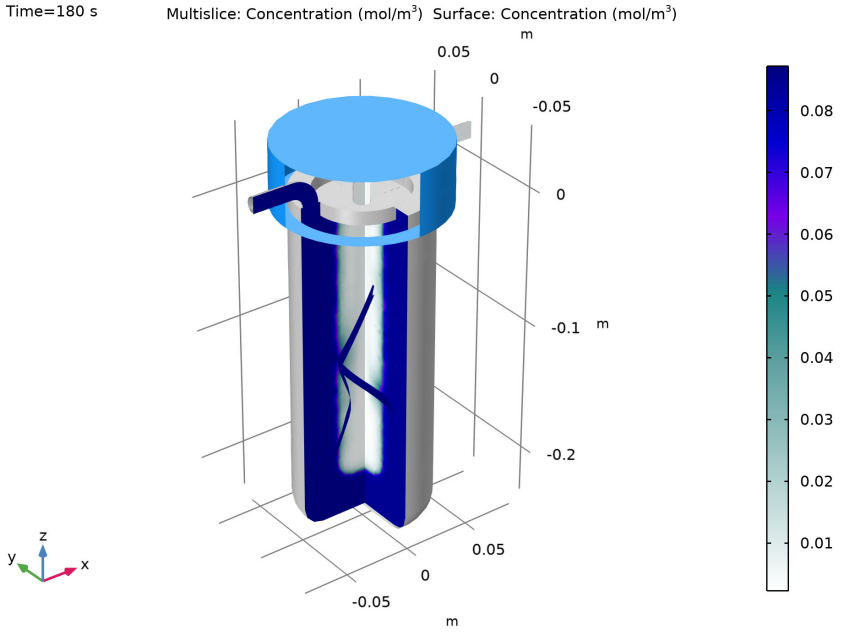


Figure 4: Chlorine concentration after 3minutes.

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.

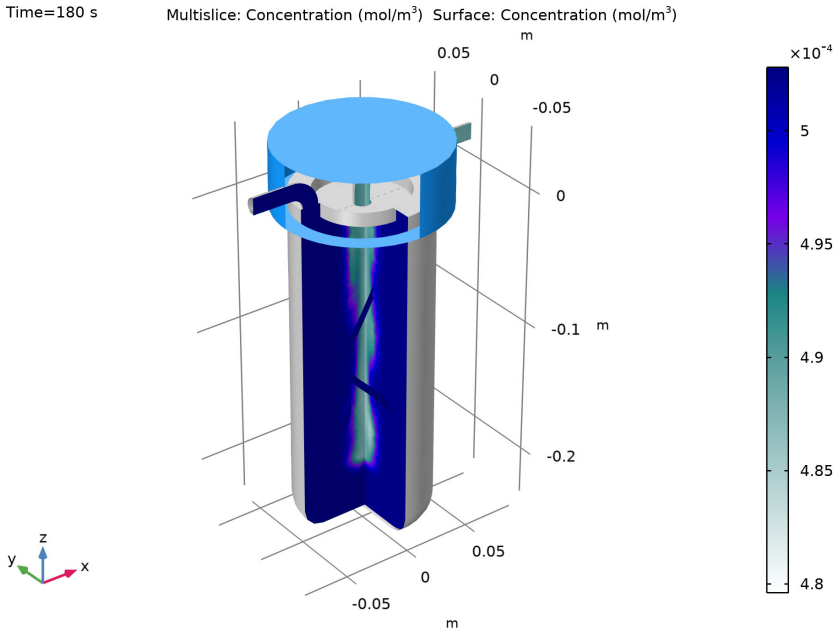


Figure 5: Chloroform concentration after 3 minutes.

The performance of the filter is evaluated by computing the ratio between the concentration at the outlet and the concentration at the inlet. The simulation is run twice, once with the influence of the crack taken into account and once without.Figure 6 shows the comparison of these results. The performance without the crack is shown with dashed

lines and the performance with the crack is shown with solid lines. It can be seen that the crack has the biggest influence on the filtering of the particles.

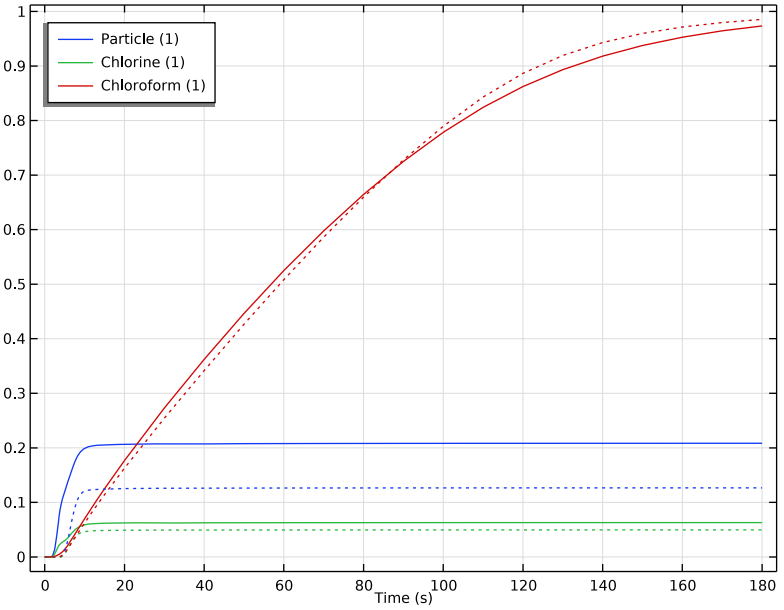


Figure 6: Effectiveness of the filter. Ratio of the concentration at the outlet to the initial concentration, with crack (solid lines) and without crack (dashed lines).

Notes About the COMSOL Implementation

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

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

Application Library path: `Porous_Media_Flow_Module/Solute_Transport/ceramic_water_filter`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **3D**.

2 In the **Select Physics** tree, select **Fluid Flow>Porous Media and Subsurface Flow>Free and Porous Media Flow, Darcy**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Chemical Species Transport>Transport of Diluted Species (tds)**.

5 Click **Add**.

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.

6 In the **Number of species** text field, type 3.

7 In the **Concentrations (mol/m³)** table, enter the following settings:

c_p
c_cl
c_chcl3

8 Click **Study**.

9 In the **Select Study** tree, select **General Studies>Stationary**.

10 Click **Done**.

GEOMETRY 1

Start importing the geometry sequence from a file. This file also includes geometry parameters and selections.

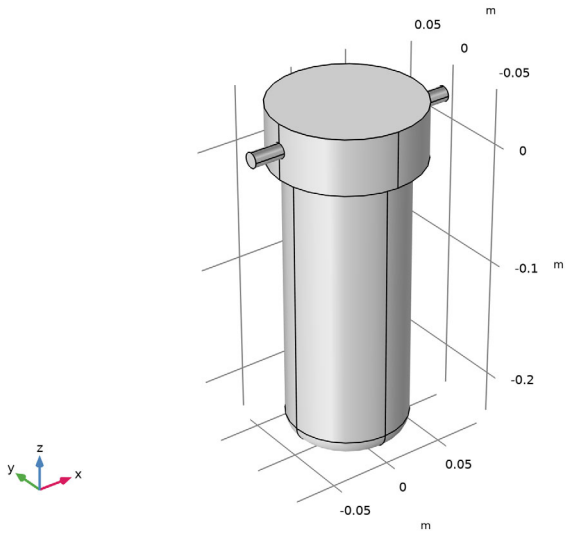
1 In the **Model Builder** window, expand the **Component 1 (comp1)>Geometry 1** node.

2 Right-click **Geometry 1** and choose **Insert Sequence**.

3 Browse to the model's Application Libraries folder and double-click the file `ceramic_water_filter_geom_sequence.mph`.

4 In the **Geometry** toolbar, click **Build All**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.



GLOBAL DEFINITIONS

Parameters: Geometry

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, type `Parameters: Geometry` in the **Label** text field.

Parameters: Transport

Now enter the parameters needed for the species transport equations and for Darcy's law. You can import the corresponding file as follows:

1 In the **Home** toolbar, click **Parameters** and choose **Add>Parameters**.

2 In the **Settings** window for **Parameters**, type `Parameters: Transport` in the **Label** text field.

3 Locate the **Parameters** section. Click **Load from File**.

4 Browse to the model's Application Libraries folder and double-click the file `ceramic_water_filter_transport_parameters.txt`.

MATERIALS

Continue with adding the materials. Water is used from the built-in material library. All other materials are user defined. Which material properties are required will be determined during the physics setup.

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

Porous Material: Ceramics

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **More Materials>Porous Material**.
2 In the **Settings** window for **Porous Material**, locate the **Geometric Entity Selection** section.
3 From the **Selection** list, choose **Ceramics**.
4 In the **Label** text field, type `Porous Material: Ceramics`.

Porous Material: Carbon

1 Right-click **Materials** and choose **More Materials>Porous Material**.
2 In the **Settings** window for **Porous Material**, locate the **Geometric Entity Selection** section.
3 From the **Selection** list, choose **Carbon**.
4 In the **Label** text field, type `Porous Material: Carbon`.

Water, liquid (mat1)

In the **Model Builder** window, right-click **Water, liquid (mat1)** and choose **Duplicate**.

Fracture

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Water, liquid 1 (mat2)**.
2 In the **Settings** window for **Material**, type `Fracture` in the **Label** text field.

3 Locate the **Geometric Entity Selection** section. From the **Geometric entity level** list, choose **Boundary**.

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

LAMINAR FLOW (SPF)

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

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.

2 In the **Settings** window for **Laminar Flow**, locate the **Domain Selection** section.

3 From the **Selection** list, choose **Laminar flow domains**.

Inlet 1

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

An inflow velocity of 0.33 m/s is assumed as inlet condition. This corresponds to a flow rate of approximately 2 l/min.

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

3 From the **Selection** list, choose **Unfiltered water inlet**.

4 Locate the **Velocity** section. In the U_0 text field, type `0.33`.

Outlet 1

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

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

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

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 **Filter domains**.

4 Click to expand the **Discretization** section. From the **Pressure** list, choose **Linear**.

Porous Medium 2

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

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

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

Porous Matrix 1

1 In the **Model Builder** window, click **Porous Matrix 1**.

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

3 From the **Permeability model** list, choose **Kozeny-Carman**.

4 In the d_p text field, type `dp_carbon`.

Fracture 1

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 **Aperture** section. In the d_f text field, type `df`.

Fracture Material 1

1 In the **Model Builder** window, click **Fracture Material 1**.

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

3 From the **Permeability model** list, choose **Cubic law**.

TRANSPORT OF DILUTED SPECIES (TDS)

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

Make sure that this interface is deactivated on the mount, and that mass transfer in porous media is enabled.

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

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

4 Locate the **Transport Mechanisms** section. Select the **Mass transfer in porous media** check box.

Transport Properties 1

1 In the **Model Builder** window, under **Component 1 (comp1)> Transport of Diluted Species (tds)** click **Transport Properties 1**.

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

3 From the **u** list, choose **Velocity field (spf)**.

Porous Medium 1

1 In the **Physics** toolbar, click **Domains** and choose **Porous Medium**.

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

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

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.

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

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

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

Porous Medium 1

In the **Model Builder** window, right-click **Porous Medium 1** and choose **Duplicate**.

Porous Medium 2

1 In the **Model Builder** window, click **Porous Medium 2**.

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 $K_{\mathrm{F,cchcl3}}$ text field, type `Kf`.

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

7 In the $c_{\mathrm{ref,cchcl3}}$ 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 1

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_cl*c_cl`.

Fracture 1

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`.

Fluid 1

1 In the **Model Builder** window, click **Fluid 1**.

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

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

Initial Values 2

To complete setting up the physics, add initial and boundary conditions for the transport equations.

1 In the **Physics** toolbar, click **Domains** and choose **Initial Values**.

2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.

3 In the c_p text field, type `c_p0`.

4 In the c_{cl} text field, type `c_cl0`.

5 In the c_{chcl3} text field, type `c_chcl30`.

6 Select Domains 1, 3, and 4 only.

Concentration 1

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_cl0`.

8 Select the **Species c_chcl3** check box.

9 In the $c_{0,cchcl3}$ text field, type `c_chcl30`.

Outflow 1

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**.

MATERIALS

Now the missing material properties can be added.

Porous Material: Ceramics (pmat1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Porous Material: Ceramics (pmat1)**.

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

3 In the ε_p text field, type `por_ceramics`.

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

Property	Variable	Value	Unit	Property group
Permeability	kappa_iso ; kappaii = kappa_iso, kappaij = 0	`kappa_ceramics`	m²	Basic

5 Locate the **Phase-Specific Properties** section. Click **Add Required Phase Nodes**.

Fluid 1 (pmat1.fluid1)

1 In the **Model Builder** window, click **Fluid 1 (pmat1.fluid1)**.

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

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

Porous Material: Carbon (pmat2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Porous Material: Carbon (pmat2)**.

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

3 In the ε_p text field, type `por_carbon`.

4 Locate the **Phase-Specific Properties** section. Click **Add Required Phase Nodes**.

Fluid 1 (pmat2.fluid1)

1 In the **Model Builder** window, click **Fluid 1 (pmat2.fluid1)**.

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

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

Solid 1 (pmat2.solid1)

1 In the **Model Builder** window, click **Solid 1 (pmat2.solid1)**.

2 In the **Settings** window for **Solid**, locate the **Solid Properties** section.

3 In the θ_s text field, type `1-por_carbon`.

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

Property	Variable	Value	Unit	Property group
Density	rho	375	kg/m³	Basic

Fracture (mat2)

1 In the **Model Builder** window, under **Component 1 (comp1)>Materials** click **Fracture (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_fracture`	1	Basic

MESH 1

Set up a proper mesh. High gradients for the concentrations are expected in the filter domains. Limit the maximum element size to resolve the geometry and these gradients properly.

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.

2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Coarse**.

4 Right-click **Component 1 (comp1)>Mesh 1** and choose **Edit Physics-Induced Sequence**.

Size 1

1 In the **Model Builder** window, right-click **Free Tetrahedral 1** and choose **Size**.

2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.

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

4 Locate the **Element Size** section. Click the **Custom** button.

5 Locate the **Element Size Parameters** section.

6 Select the **Maximum element size** check box. In the associated text field, type `th_ceramics/2`.

7 Select the **Minimum element size** check box. In the associated text field, type `th_ceramics/4`.

8 Select the **Curvature factor** check box. In the associated text field, type `0.2`.

Boundary Layers 2

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 Select Boundaries 31–34, 51, 52, 71, 72, 78, 85, 93, and 97 only.

3 In the **Settings** window for **Boundary Layer Properties**, locate the **Layers** section.

4 In the **Number of layers** text field, type `4`.

5 From the **Thickness specification** list, choose **First layer**.

6 In the **Thickness** text field, type `th_ceramics/20`.

Free Tetrahedral 2

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

2 In the **Settings** window for **Free Tetrahedral**, click  **Build All**.

STUDY 1

The simulation should take 3 minutes. Within this time interval the flow can be regarded as independent of the concentration.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 In the table, enter the following settings:

Physics interface	Solve for	Equation form
Transport of Diluted Species (tds)		Automatic (Stationary)

4 In the **Model Builder** window, click **Study 1**.

5 In the **Settings** window for **Study**, locate the **Study Settings** section.

6 Clear the **Generate default plots** check box.

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

Step 2: 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 boxes for **Laminar Flow (spf)** and **Darcy's Law (dl)**.

4 In the table, clear the **Solve for** check box for **Free and Porous Media Flow Coupling 1 (nsd1)**.

5 Locate the **Study Settings** section. In the **Output times** text field, type `range(0,0.5,15) range(20,10,180)`.

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 dynamics caused by the applied discontinuous initial concentrations.

Step 1: Stationary

In order to compare the performance of the filter with and without the crack, the simulation is first run with the effect of the fracture disabled.

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the tree, select **Component 1 (comp1)>Darcy's Law (dl)>Fracture 1**.

5 Click **Disable**.

Step 2: Time Dependent

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Select the **Modify model configuration for study step** check box.

4 In the tree, select **Component 1 (comp1)>Transport of Diluted Species (tds)>Fracture 1**.

5 Click **Disable**.

6 In the **Study** toolbar, click **Compute**.

RESULTS

The performance of the filter without the crack is recorded in a table by computing the ratio between the concentration at the outlet and the concentration at the inlet.

Surface Average 1

1 In the **Model Builder** window, expand the **Results** node.

2 Right-click **Results>Derived Values** and choose **Average>Surface Average**.

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

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

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

Expression	Unit	Description
c_p/c_p0	1	Particle
c_cl/c_cl0	1	Chlorine
c_chcl3/c_chcl30	1	Chloroform

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

STUDY 1

For the next computation, enable again the effect of the fracture.

Step 1: Stationary

1 In the **Model Builder** window, under **Study 1** click **Step 1: Stationary**.

2 In the **Settings** window for **Stationary**, locate the **Physics and Variables Selection** section.

3 Clear the **Modify model configuration for study step** check box.

Step 2: Time Dependent

1 In the **Model Builder** window, click **Step 2: Time Dependent**.

2 In the **Settings** window for **Time Dependent**, locate the **Physics and Variables Selection** section.

3 Clear the **Modify model configuration for study step** check box.

4 In the **Home** toolbar, click **Compute**.

Create new datasets to use for visualizing the geometry.

RESULTS

Surface 1

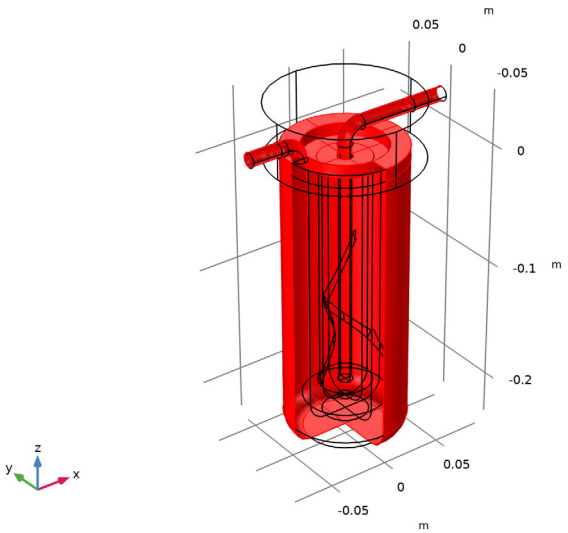
1 In the **Results** toolbar, click **More Datasets** and choose **Surface**.

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

3 Click **Paste Selection**.

4 In the **Paste Selection** dialog box, type `4, 5, 10, 12, 17, 18, 20, 22, 24, 26, 30, 35-38, 48, 49, 60, 63, 66-70, 73, 74, 77, 84, 90-92, 95, 96, 98-101, 107, 108, 111, 112` in the **Selection** text field.

5 Click **OK**.



6 Right-click **Surface 1** and choose **Duplicate**.

Surface 2

1 In the **Model Builder** window, click **Surface 2**.

2 Select Boundaries 7, 8, 13, 65, and 102 only.

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 **Expression** section.
3. In the **Expression** text field, type `p`.
4. Locate the **Multiplane Data** section. Find the **z-planes** subsection. In the **Planes** text field, type `0`.
5. Right-click **Multislice 1** and choose **Duplicate**.

Multislice 2

1. In the **Model Builder** window, click **Multislice 2**.
2. In the **Settings** window for **Multislice**, locate the **Expression** section.
3. In the **Expression** text field, type `p2`.
4. Click to expand the **Inherit Style** section. From the **Plot** list, choose **Multislice 1**.

Surface 1

1. In the **Model Builder** window, right-click **Pressure** and choose **Surface**.
2. In the **Settings** window for **Surface**, locate the **Expression** section.
3. In the **Expression** text field, type `p2`.
4. Click to expand 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 **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**.

8 Right-click **Surface 2** and choose **Duplicate**.

Surface 3

1 In the **Model Builder** window, click **Surface 3**.

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

3 From the **Dataset** list, choose **Surface 2**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Custom**.

5 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

6 Click **Define custom colors**.

7 Set the RGB values to 18, 145, and 243, respectively.

8 Click **Add to custom colors**.

9 Click **Show color palette only** or **OK** on the cross-platform desktop.

10 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 **Multiplane Data** section. Find the **z-planes** subsection. In the **Planes** text field, type `0`.

5 Locate the **Coloring and Style** section. Click **Change Color Table**.

6 In the **Color Table** dialog box, select **Aurora>AuroraAustralis** in the tree.

7 Click **OK**.

8 In the **Settings** window for **Multislice**, click to expand the **Quality** section.

9 From the **Recover** list, choose **Everywhere**.

10 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**.

8 Right-click **Surface 2** and choose **Duplicate**.

Surface 3

1 In the **Model Builder** window, click **Surface 3**.

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

3 From the **Dataset** list, choose **Surface 2**.

4 Locate the **Coloring and Style** section. From the **Color** list, choose **Custom**.

5 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.

6 Click **Define custom colors**.

7 Set the RGB values to 18, 145, and 243, respectively.

8 Click **Add to custom colors**.

9 Click **Show color palette only** or **OK** on the cross-platform desktop.

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**.

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

5 Right-click **Particle concentration** and choose **Duplicate**.

Chlorine concentration

1 In the **Model Builder** window, under **Results** click **Particle concentration 1**.

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_cl`.

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_cl`.

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

Duplicate this plot again and repeat the steps to plot the chloroform concentration `c_chcl3`. Compare with Figure 5.

Surface Average 1

Finally, create Figure 6.

In the **Model Builder** window, under **Results>Derived Values** right-click **Surface Average 1** and choose **Evaluate>New Table**.

TABLE 2

1 Go to the **Table 2** window.

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

RESULTS

Table Graph 1

1. In the **Model Builder** window, under **Results>1D 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 **1D Plot Group 5**.
2. In the **Settings** window for **1D Plot Group**, type `Concentration over time.` in the **Label** text field.
3. Locate the **Legend** section. From the **Position** list, choose **Upper left**.

Table Graph 1

In the **Model Builder** window, right-click **Table Graph 1** and choose **Duplicate**.

Table Graph 2

1. In the **Model Builder** window, click **Table Graph 2**.
2. In the **Settings** window for **Table Graph**, locate the **Data** section.
3. From the **Table** list, choose **Table 1**.
4. Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Line** list, choose **Dotted**.
5. From the **Color** list, choose **Cycle (reset)**.
6. Locate the **Legends** section. Clear the **Show legends** check box.
7. In the **Concentration over time.** toolbar, click  **Plot**.