



Protein Adsorption

This application simulates an ion-exchange column for protein adsorption. The fluid phase contains four components: two proteins, one solvent, and one salt. The adsorption/desorption kinetics is described by two equilibrium reactions where proteins displace ions adsorbed at the surface and vice versa.

The example highlights how reactions at chemical equilibrium can be studied in a 0D reactor system in Reaction Engineering. In addition, it also shows how the kinetics from the 0D setup is exported to a 3D model where the reacting surface in the column can be studied in detail. The 3D model incorporates mass transport through diffusion and convection, and the reactions at the surface of the ion-exchange mass with Transport of Diluted Species, Laminar Flow, and Surface Reactions interfaces.

Introduction Protein Ion-Exchange

The binding of proteins to ion exchangers can be described within the steric mass action approximation (SMA). This approach assumes that the adsorption of a protein can be considered as an exchange reaction of the protein with a given number of adsorbed ions, the process is schematically depicted in [Figure 1](#).

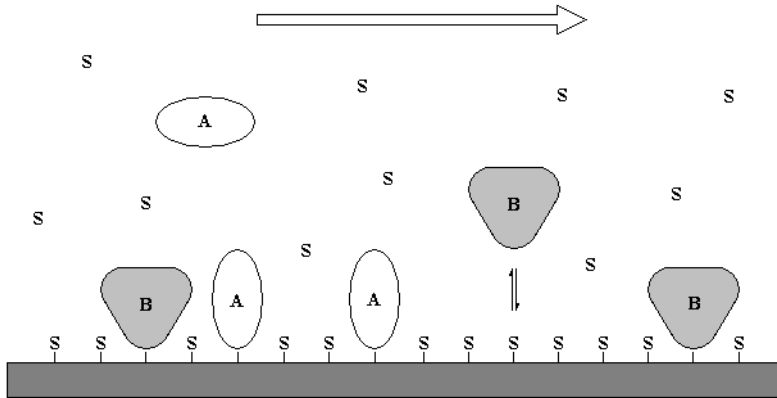


Figure 1: Proteins A and B displacing salt ions S at an ion-exchanger surface.

The equilibrium describing the adsorption/desorption reactions is



Here, S denotes the salt ion, P stands for either protein A and B. Once P is adsorbed, P(ads), salt ions are displaced, reducing the concentration of adsorbed salt ions, S(ads).

Model Definition

The system is modeled both in 0D and in 3D. The former model setup is adequate to investigate the kinetics of the equilibrium reactions within the column. The latter makes it possible to study the surface of the ion-exchange beads that make up the porous structure of the ion-exchange mass. In Figure 2, the two model approaches are presented.

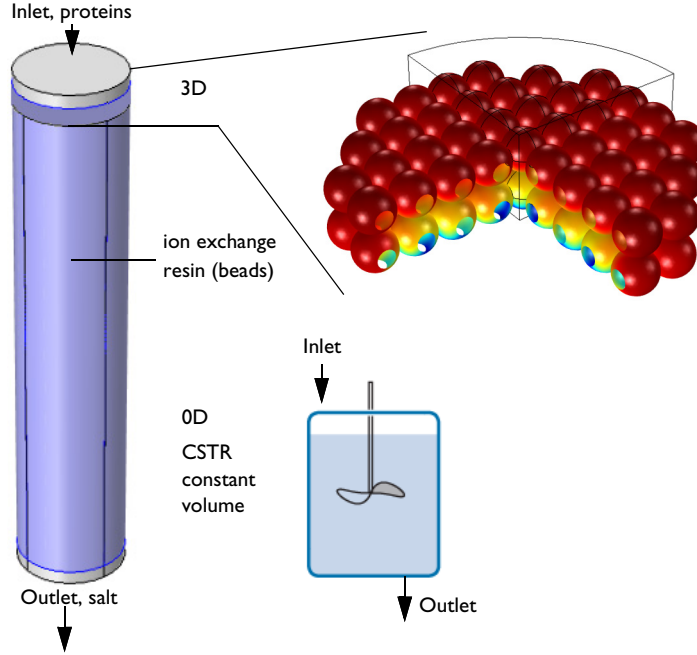


Figure 2: Ion-exchange column and model geometries. The 0D model approximates the entire column, while the 3D geometry is a detailed representation of a section at the top of the column.

The 0D model utilizes the reactor type CSTR, constant volume in the Reaction Engineering interface. Ideal conditions are assumed within the reactor, meaning that well-mixed conditions with no concentration gradients apply. The reaction kinetics are described by Equation 1 for proteins A and B are entered directly into the interface as equilibrium surface reactions. The equilibrium constants for reaction 1, adsorption of A, is $K_1^{\text{eq}} = 2$ and for reaction 2, adsorption of B, is $K_2^{\text{eq}} = 5$. These are entered as well, relating the concentrations as followed

$$K_1^{\text{eq}} = \frac{c_S c_{A(\text{ads})}}{c_A c_{S(\text{ads})}} \quad (2)$$

$$K_2^{c_q} = \frac{c_S c_{B(ads)}}{c_B c_{S(ads)}} \quad (3)$$

In order to compute the concentrations, both protein surface concentrations need to be set as dependent in the Equilibrium Species Vector section.

The proteins enter the reactor with a Feed Inlet with concentrations that vary in accordance to a 10 s Gaussian pulse with a maximum of 0.05 mol/m^3 . The outlet flow rate regulates so that the volume of the reactor is constant. Initially, no protein is available in the column and the ion-exchange mass is set to be completely adsorbed with salt, that is, the initial site density, γ_0 , is equal to the initial surface concentration of S, $S(ads)$.

For the 3D model, as shown in [Figure 3](#), only one quarter of the top section of the column is simulated due to symmetry. The proteins enter the top with a constant concentration of 0.05 mol/m^3 . In the column initially, the pores (the bulk) is filled with solvent and the ion-exchange beads are saturated with adsorbed salt.

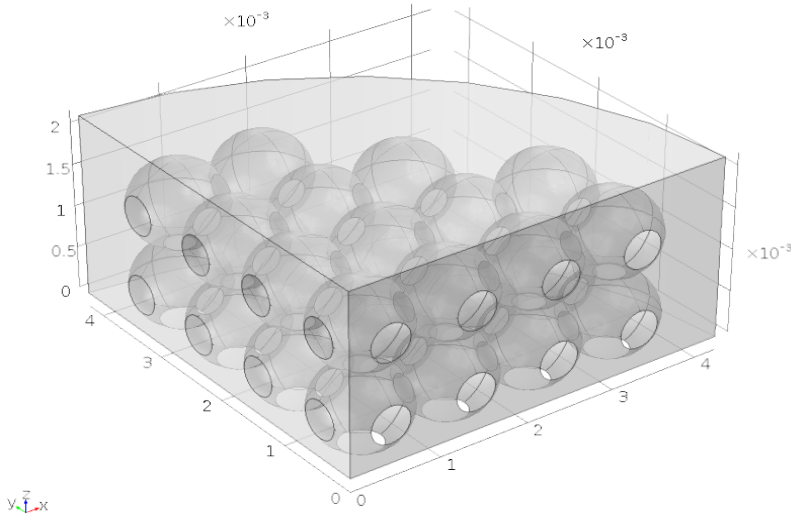


Figure 3: 3D model geometry.

The reaction kinetics are taken directly from the 0D model with the Generate Space-Dependent Model feature and are collected in a Chemistry interface that also supplies computed diffusion coefficients and fluid density for the 3D setup.

The mass balances describing the species mass transport in the pores of the column are set up with the Transport of Diluted Species interface with diffusion and convection accounted for

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (-D_i \nabla c_i) + u \cdot \nabla c_i = 0 \quad (4)$$

On the right hand side of [Equation 4](#) no reaction source is present for the bulk. However, the surface of the ion-exchange beads produces a reaction source that needs to be coupled to this equation. This is simply done with a Surface Reaction interface. Such an interface is automatically generated with the use of the Generate Space-Dependent Model feature if surface reactions are present.

The 3D model also computes the convective velocity, u , with a Laminar Flow interface. The velocity is based on the assumption that the velocity, U , within the reactor is 0.1 mm/s and that the inlet is open to the surroundings, that is, exposed to the atmospheric pressure.

STUDY SETTINGS

The 3D problem is solved in a two-step study. First, the Laminar Flow interface is first solved with a Stationary study step. Second, the rest of the interfaces (Chemistry, Transport of Diluted Species, and Surface Reactions) are solved with a Time Dependent study step. A Fully Coupled Direct solver is required in the second step to obtain stable computations.

Study 1 — Space Independent

[Figure 4](#) shows how the concentrations of the reacting species change with the time. Initially, only adsorbed salt species are present in the column. The concentrations of proteins A and B are seen to change with the Gaussian concentration pulse feed inlet. A stronger adsorption affinity of protein B compared to protein A is readily observed. Note also how the concentration of bulk salt species S increases as the proteins adsorb at the

surface. Toward the end of the pulse, most proteins have been adsorbed in the column and the bulk salt species have exited the system.

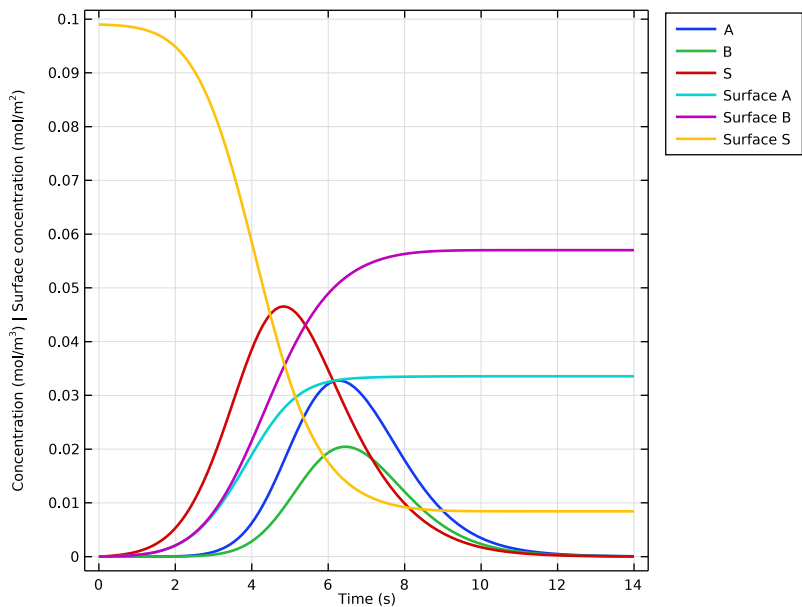


Figure 4: Concentrations of the reacting species as functions of time (s).

Study 2 — Space Dependent

The 3D model is solved for 30 s and a selection of the results are displayed in this section. [Figure 5](#), [Figure 6](#), [Figure 7](#), and [Figure 8](#) show the behavior of protein B after 5 s and 30 s.

From [Figure 6](#), in which the bulk concentration is shown, indicates that the beads at the center of the column are less accessible for adsorption or that the protein is more rapidly adsorbed at the center, both phenomena lowering the bulk concentration there.

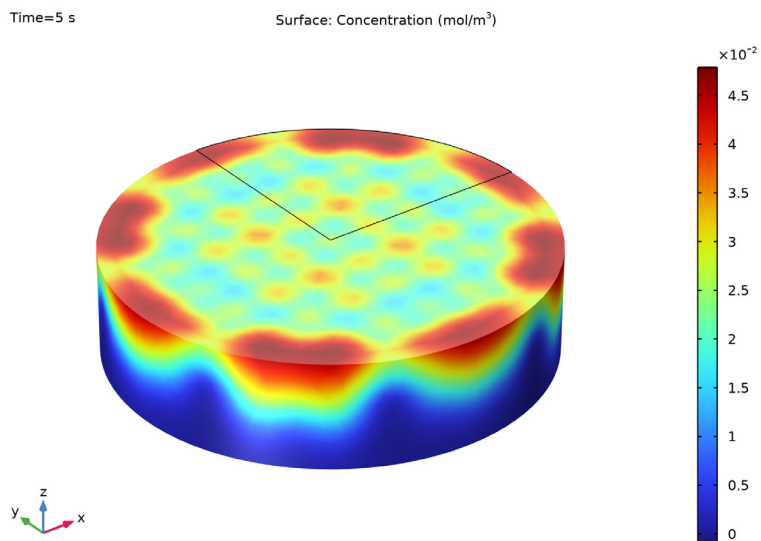


Figure 5: Bulk concentration of B at 5 s.

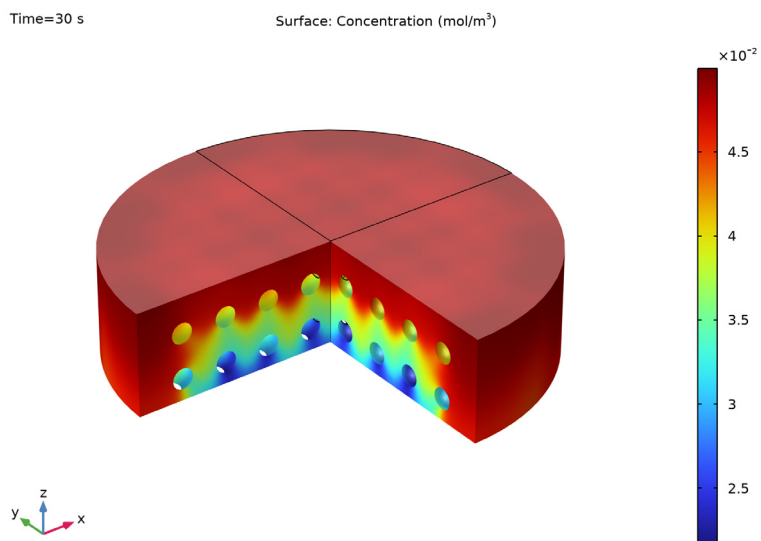


Figure 6: Bulk concentration of B at 30 s.

To get a proper understanding of the ion-exchange beads, a comparison of the adsorbed B surface concentration at the two times is also made with the results in [Figure 7](#) and [Figure 8](#). The lower surface concentration of B in the center suggests that less B is adsorbed there and that the porous structure obstructs the species transport. Note that the bead surface cannot adsorb more than the (initial) site density of the ion-exchange material, γ_0 (SI unit: mol/m²).

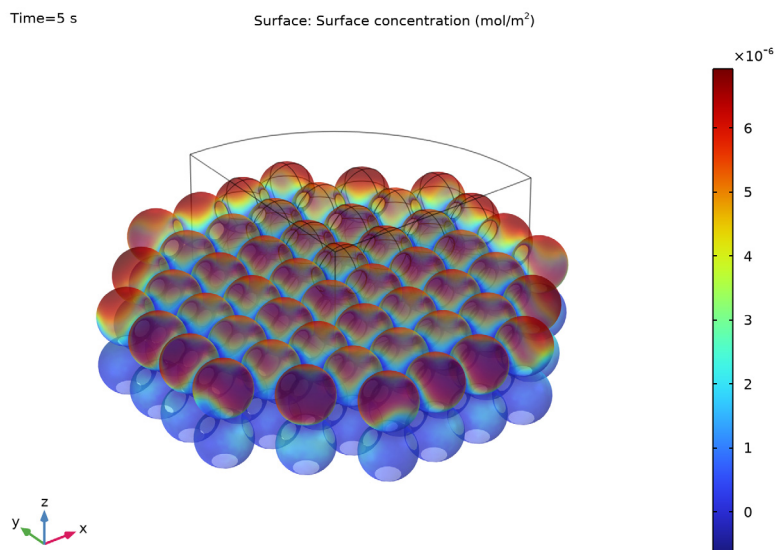


Figure 7: Surface concentration of B at 5 s.

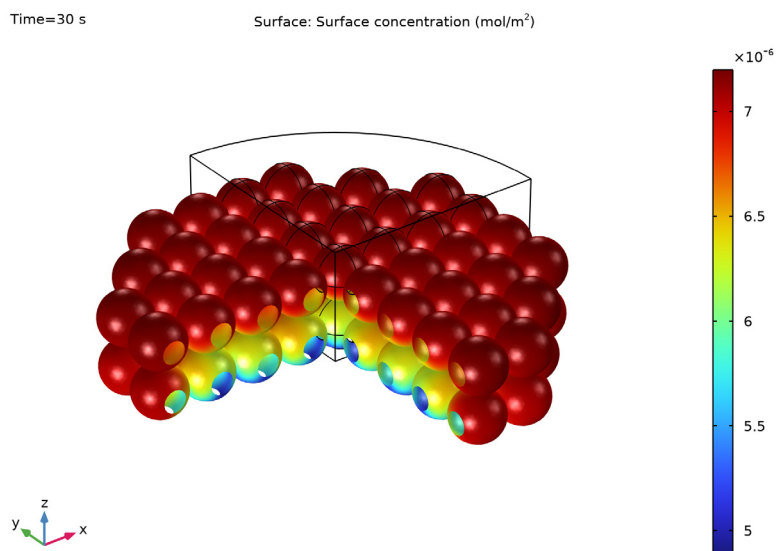


Figure 8: Surface concentration of B at 30 s.

In Figure 9, the velocity field is displayed. It shows that the porous structure causes a quite distorted velocity field. The exception is at the walls where the flow is less obstructed due to the relatively large gap between beads and wall.

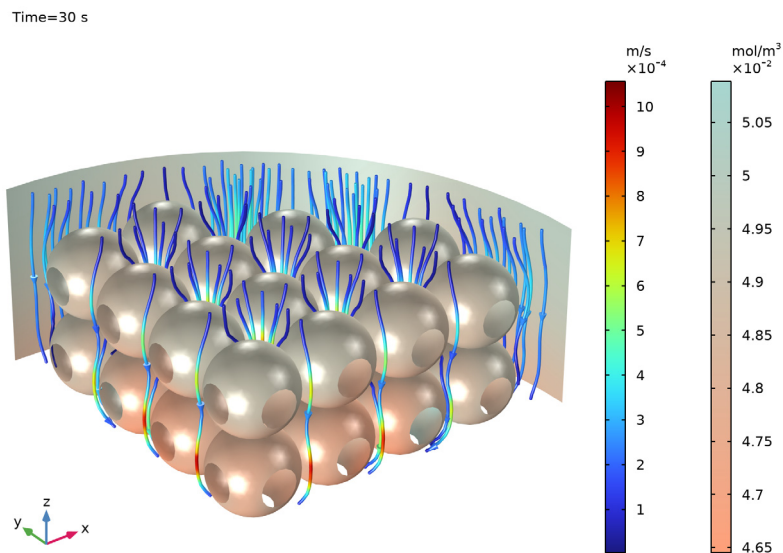



Figure 9: Velocity field in the pores of the column section.

Application Library path: Chemical_Reaction_Engineering_Module/
Mixing_and_Separation/protein_adsorption


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  **1D**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport>Reaction Engineering (re)**.

- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **General Studies>Time Dependent**.
- 6 Click  **Done**.

GLOBAL DEFINITIONS


Import the model parameters from a file from the application's **Application Library** folder.

Parameters I

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 2 In the **Settings** window for **Parameters**, locate the **Parameters** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `protein_adsorption_parameters.txt`.

Gaussian Pulse I (gpI)

Reactants are injected to the system in a pulse. Choose a **Gaussian Pulse** function to describe the injection.

- 1 In the **Home** toolbar, click  **Functions** and choose **Global>Gaussian Pulse**.
- 2 In the **Settings** window for **Gaussian Pulse**, locate the **Parameters** section.
- 3 In the **Location** text field, type 5.
- 4 In the **Standard deviation** text field, type 1.5.

Use the **Gaussian Pulse** function to set up a time-dependent pulse variable with an amplitude of 1.

DEFINITIONS

Variables I

- 1 In the **Model Builder** window, under **Component I (compI)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 In the table, enter the following settings:

Name	Expression	Unit	Description
pulse11	$3.76 * gp1(t/1[s])$		Pulse with amplitude 1


REACTION ENGINEERING (RE)

Select a constant volume CSTR to model the ion-exchange column in 0D.

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Reaction Engineering (re)**.
- 2 In the **Settings** window for **Reaction Engineering**, locate the **Reactor** section.
- 3 From the **Reactor type** list, choose **CSTR, constant volume**.
- 4 Locate the **Mixture Properties** section. From the **Phase** list, choose **Liquid**.

Reaction 1

Set up the equilibrium reaction for adsorption/desorption of protein A.

- 1 In the **Reaction Engineering** toolbar, click  **Reaction**.
- 2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.
- 3 In the **Formula** text field, type $S(ads) + A = S + A(ads)$.
- 4 Click **Apply**.
- 5 Locate the **Equilibrium Settings** section. In the K_j text field, type K_{eq01} .

Enter densities and molar masses in the bulk species nodes for **Reaction 1**.

Surface species: S(ads)

COMSOL will automatically assign the S to be sulfur. However, in this case is S a descriptive variable for the salt ion.

- 1 In the **Model Builder** window, click **Surface species: S(ads)**.
- 2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.
- 3 Clear the **Enable formula** check box.
- 4 In the M text field, type MS.

Species: A

- 1 In the **Model Builder** window, click **Species: A**.
- 2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.
- 3 In the M text field, type MA.
- 4 In the ρ text field, type ρ_{0p} .

Species: S

- 1 In the **Model Builder** window, click **Species: S**.
- 2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.
- 3 Clear the **Enable formula** check box.
- 4 In the M text field, type MS.

5 In the ρ text field, type ρ_{S} .

Surface species: A(ads)

1 In the **Model Builder** window, click **Surface species: A(ads)**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 In the M text field, type MA.

Reaction 2

1 In the **Reaction Engineering** toolbar, click  **Reaction**.

In similar fashion, set up the equilibrium reaction for adsorption/desorption of protein B.

2 In the **Settings** window for **Reaction**, locate the **Reaction Formula** section.

3 In the **Formula** text field, type $\text{S(ads)} + \text{B} = \text{S} + \text{B(ads)}$.

4 Click **Apply**.

5 Locate the **Equilibrium Settings** section. In the K_j text field, type K_{eq02} .

As before, enter densities and molar masses in the bulk species nodes, but now for **Reaction 2**.

Species: B

Similar to S, B does not represent boron in this case, but is instead a descriptive variable of protein B.

1 In the **Model Builder** window, click **Species: B**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Clear the **Enable formula** check box.

4 In the M text field, type MB.

5 In the ρ text field, type ρ_{p} .

Surface species: B(ads)

1 In the **Model Builder** window, click **Surface species: B(ads)**.

2 In the **Settings** window for **Species**, locate the **Chemical Formula** section.

3 Clear the **Enable formula** check box.

4 In the M text field, type MB.

Replace the default dependent variables and replace these with **A(ads)** and **B(ads)**. This omits any cyclic dependence of the reaction rates.

5 In the **Model Builder** window, click **Reaction Engineering (re)**.

- 6 In the **Settings** window for **Reaction Engineering**, locate the **Equilibrium Species Vector** section.
- 7 In the **Predefined dependent species (separated by ':')** text field, type A(ads) : B(ads).
- 8 Locate the **Reactor** section. Find the **Mass balance** subsection. From the **Volumetric rate** list, choose **User defined**.
Set $v_p=0$, to neglect the volumetric production rate.
- 9 In the v_p text field, type 0.
Select the reactive surface area available in the reactor. This regulates, when multiplied with the site density, how much the ion-exchange column can adsorb.
- 10 Find the **Surface reaction area** subsection. In the A_r text field, type A_{rsurf} .

Initial Values I


In the **Initial Values** feature, set all species except adsorbed S (**S(ads)**) to zero. Also, set the initial density of surface sites for the ion-exchange mass. Note that the latter property sets the upper limit of how many moles can be adsorbed. Assume that each species takes up one reactive site.

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, click to expand the **Surface Species Initial Values** section.
- 3 In the Γ_s text field, type G0.
- 4 In the table, enter the following settings:

Species	Surface concentration (mol/m ²)	Site occupancy number (I)
S(ads)	CS0surf	1

Feed Inlet I

Last, in the OD model, add the **Feed Inlet** feature containing bulk species A and B. Add the concentration with the Gaussian pulse in the feed stream.

- 1 In the **Reaction Engineering** toolbar, click  **Feed Inlet**.
- 2 In the **Settings** window for **Feed Inlet**, locate the **Feed Inlet Properties** section.
- 3 In the v_f text field, type v_{fp} .

- 4 Locate the **Feed Inlet Concentration** section. In the **Feed inlet concentration** table, enter the following settings:


Species	Concentration (mol/m ³)
A	C _{Amax_inlet} *pulse11
B	C _{Bmax_inlet} *pulse11

Solve the 0D model for 14 s.

STUDY 1 - SPACE INDEPENDENT

- 1 In the **Model Builder** window, click **Study 1**.
- 2 In the **Settings** window for **Study**, type Study 1 - Space Independent in the **Label** text field.

Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study 1 - Space Independent** click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 In the **Output times** text field, type range(0,0.1,14).
- 4 In the **Home** toolbar, click  **Compute**.

RESULTS

Concentrations 0D model

Create [Figure 4](#) in which all species concentrations are displayed.

- 1 In the **Settings** window for **ID Plot Group**, type Concentrations 0D model in the **Label** text field.
- 2 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 3 Locate the **Plot Settings** section. Select the **x-axis label** check box.
- 4 Select the **y-axis label** check box. In the associated text field, type Concentration (mol/m³) | Surface concentration (mol/m²).
- 5 Locate the **Legend** section. From the **Layout** list, choose **Outside graph axis area**.

Global 1

- 1 In the **Model Builder** window, expand the **Concentrations 0D model** node, then click **Global 1**.

- 2 In the **Settings** window for **Global**, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.c_A - Concentration - mol/m³**.
- 3 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.c_B - Concentration - mol/m³**.
- 4 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.c_S - Concentration - mol/m³**.
- 5 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.csurf_A_surf - Surface concentration - mol/m²**.
- 6 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.csurf_B_surf - Surface concentration - mol/m²**.
- 7 Click **Add Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Component I (compI)>Reaction Engineering>re.csurf_S_surf - Surface concentration - mol/m²**.
- 8 Locate the **y-Axis Data** section. In the table, enter the following settings:

Expression	Unit	Description
re.csurf_A_surf*1e4	mol/m ²	Surface concentration per square dm
re.csurf_B_surf*1e4	mol/m ²	Surface concentration per square dm
re.csurf_S_surf*1e4	mol/m ²	Surface concentration per square dm

- 9 Click to expand the **Coloring and Style** section. From the **Width** list, choose **2**.
- 10 Click to expand the **Legends** section. From the **Legends** list, choose **Manual**.
- 11 In the table, enter the following settings:

Legends
A
B
S
Surface A


Legends
Surface B
Surface S

12 In the **Concentrations 0D model** toolbar, click  **Plot**.

Continue setting up a space-dependent model to investigate the top section of the ion-exchange column. Start by adding a solvent to the system. The solvent in these types of systems is often water.

REACTION ENGINEERING (RE)

Species I

- 1** In the **Reaction Engineering** toolbar, click  **Species**.
- 2** In the **Settings** window for **Species**, locate the **Name** section.
- 3** In the text field, type H2O.
- 4** Locate the **Type** section. From the list, choose **Solvent**.
- 5** Locate the **Chemical Formula** section. In the M text field, type MH2O.
- 6** In the ρ text field, type rho_H2O.

Initial Values I

- 1** In the **Model Builder** window, click **Initial Values I**.
- 2** In the **Settings** window for **Initial Values**, locate the **Volumetric Species Initial Values** section.
- 3** In the table, enter the following settings:


Species	Concentration (mol/m ³)
H2O	CH2O

Specify the transport properties of the solvent. These will be transferred to the **Chemistry** interface in the space-dependent model below.

- 4** In the **Model Builder** window, click **Reaction Engineering (re)**.
- 5** In the **Settings** window for **Reaction Engineering**, click to expand the **Calculate Transport Properties** section.
- 6** Select the **Calculate mixture properties** check box.
- 7** From the **Dynamic viscosity** list, choose **User defined**.
- 8** In the μ text field, type muH2O.



Use the **Generate Space-dependent Model** feature. Select to create a 3D geometry together with a **Transport of Diluted Species** and a **Laminar Flow** interface and a **Time Dependent** study type.

Generate Space-Dependent Model |

- 1 In the **Reaction Engineering** toolbar, click  **Generate Space-Dependent Model**.
- 2 In the **Settings** window for **Generate Space-Dependent Model**, locate the **Study Type** section.
- 3 From the **Study type** list, choose **Time dependent**.
- 4 Locate the **Physics Interfaces** section. Find the **Fluid flow** subsection. From the list, choose **Laminar Flow: New**.
- 5 Locate the **Space-Dependent Model Generation** section. Click **Create/Refresh**.

GEOMETRY 1 (3D)

Insert the 3D geometry sequence file `protein_adsorption_geom_sequence.mph` from the application's **Application Library** folder.

- 1 In the **Model Builder** window, expand the **Component 2 (comp2)** node, then click **Geometry 1(3D)**.
- 2 In the **Geometry** toolbar, click **Insert Sequence** and choose **Insert Sequence**.
- 3 Browse to the model's Application Libraries folder and double-click the file `protein_adsorption_geom_sequence.mph`.
- 4 In the **Geometry** toolbar, click  **Build All**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

TRANSPORT OF DILUTED SPECIES (TDS)

Start with the **Transport of Diluted Species** interface.

Transport Properties |

The **Laminar Flow** interface is Coupled to the velocity field.

A and B enter the column at the top. Select **Danckwerts (Flux)** for a more stable computation.

Despite the fact that only solvent makes up the fluid within the column initially, adding initial trace concentrations of all dependent species gives a more stable solution to the equilibrium reactions.

Initial Values 1

- 1 In the **Model Builder** window, expand the **Component 2 (comp2)>Transport of Diluted Species (tds)** node, then click **Initial Values 1**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the cA text field, type $CA_{\text{max_inlet}}*0.01$.
- 4 In the cB text field, type $CB_{\text{max_inlet}}*0.01$.
- 5 In the cS text field, type $1e-7$.

Inflow 1

- 1 In the **Model Builder** window, click **Inflow 1**.
- 2 In the **Settings** window for **Inflow**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.
- 4 Locate the **Concentration** section. In the $c_{0,cA}$ text field, type $CA_{\text{max_inlet}}$.
- 5 In the $c_{0,cB}$ text field, type $CB_{\text{max_inlet}}$.
- 6 Locate the **Boundary Condition Type** section. From the list, choose **Flux (Danckwerts)**.

Outflow 1

Set an **Outflow** condition at the bottom of the geometry. This means that the transport along the z direction (the height) of the reactor is dominated by convection.

- 1 In the **Model Builder** window, click **Outflow 1**.
- 2 In the **Settings** window for **Outflow**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet column section**.

Surface Equilibrium Reaction 1

The surface of the beads is the boundary where reactions take place.

- 1 In the **Model Builder** window, click **Surface Equilibrium Reaction 1**.
- 2 In the **Settings** window for **Surface Equilibrium Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Array 1**.

Surface Equilibrium Reaction 2

- 1 In the **Model Builder** window, click **Surface Equilibrium Reaction 2**.
- 2 In the **Settings** window for **Surface Equilibrium Reaction**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Array 1**.

SURFACE REACTIONS I (SR)

In the surface reactions interface make sure that the reactions take place on the surface of the beads.

- 1 In the **Model Builder** window, under **Component 2 (comp2)** click **Surface Reactions I (sr)**.
- 2 In the **Settings** window for **Surface Reactions**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Array 1**.

Reactions I

- 1 In the **Model Builder** window, expand the **Surface Reactions I (sr)** node, then click **Reactions I**.
- 2 In the **Settings** window for **Reactions**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Array 1**.

For the same reason as in the **Transport of Diluted Species** interface, add initial trace concentrations of species A and B.

Initial Values I

- 1 In the **Model Builder** window, click **Initial Values I**.
- 2 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 3 In the cs_A text field, type $CS0_{surf} * 0.01$.
- 4 In the cs_B text field, type $CS0_{surf} * 0.01$.

LAMINAR FLOW I (SPF)

At the inlet, or the top of the column, atmospheric pressure is applied since the column is open to the surroundings.

Inlet I

- 1 In the **Model Builder** window, expand the **Laminar Flow I (spf)** node, then click **Inlet I**.
- 2 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Inlet**.
- 4 Locate the **Boundary Condition** section. From the list, choose **Pressure**.


The average velocity through the xy -plane of the geometry is assumed to be constant everywhere along the column height. Set a constant velocity within the column, in this case, at the bottom of the 3D model geometry.

Outlet I


- 1 In the **Model Builder** window, click **Outlet I**.

- 2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.
- 3 From the **Selection** list, choose **Outlet column section**.
- 4 Locate the **Boundary Condition** section. From the list, choose **Velocity**.
- 5 Locate the **Velocity** section. In the U_0 text field, type `U_column`.

Symmetry I


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

Wall I

- 1 In the **Model Builder** window, click **Wall I**.
- 2 In the **Settings** window for **Wall**, locate the **Boundary Selection** section.
- 3 Click  **Create Selection**.
- 4 In the **Create Selection** dialog box, type `Walls` in the **Selection name** text field.
- 5 Click **OK**.

MULTIPHYSICS


Reacting Flow, Diluted Species I (rfdI)

In the **Physics** toolbar, click  **Multiphysics Couplings** and choose **Domain>Reacting Flow, Diluted Species**.

MESH I

Select a mesh that resolves the surface of the beads well.


Free Triangular I

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

Size I

- 1 Right-click **Free Triangular I** 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.
- 5 Select the **Maximum element size** check box. In the associated text field, type `9E-2`.

Free Tetrahedral I

- 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 **All domains**.

Size I


- 1 Right-click **Free Tetrahedral I** 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.
- 5 Select the **Maximum element size** check box. In the associated text field, type 5E-1.

This model requires that a two-step study node is used. The first step solves the stationary solution of the **Laminar Flow** interface and the second the time-dependent solution for the rest of the interfaces.

STUDY 2 - SPACE DEPENDENT

- 1 In the **Model Builder** window, click **Study 2**.
- 2 In the **Settings** window for **Study**, type Study 2 - Space Dependent in the **Label** text field.

Stationary - Laminar Flow

- 1 In the **Study** toolbar, click  **Study Steps** and choose **Stationary>Stationary**.
- 2 In the **Settings** window for **Stationary**, type Stationary - Laminar Flow in the **Label** text field.
- 3 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check boxes for **Reaction Engineering (re)**, **Chemistry I (chem)**, **Transport of Diluted Species (tds)**, and **Surface Reactions I (sr)**.

Time Dependent - the Rest of the Interfaces

- 1 In the **Model Builder** window, click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, type Time Dependent - the Rest of the Interfaces in the **Label** text field.
- 3 Locate the **Study Settings** section. In the **Output times** text field, type range(0,1,30).
- 4 From the **Tolerance** list, choose **User controlled**.
- 5 In the **Relative tolerance** text field, type 2e-4.

- 6 Locate the **Physics and Variables Selection** section. In the table, clear the **Solve for** check box for **Laminar Flow I (spf)**.


Step 2: Stationary - Laminar Flow

In the **Model Builder** window, right-click **Step 2: Stationary - Laminar Flow** and choose **Move Up**.

Solution 2 (sol2)

- 1 In the **Study** toolbar, click  **Show Default Solver**.



Replace the **Segregated** solver with a **Fully Coupled** one since this fits the quick shifts in concentration originating from the equilibrium reactions in the system. Also apply a **Direct** solver to further improve the stability of the computations.

- 2 In the **Model Builder** window, expand the **Solution 2 (sol2)** node, then click **Time-Dependent Solver I**.
- 3 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Absolute Tolerance** section.
- 4 From the **Tolerance method** list, choose **Manual**.
- 5 In the **Absolute tolerance** text field, type $1e-4$.
- 6 Right-click **Study 2 - Space Dependent>Solver Configurations>Solution 2 (sol2)>Time-Dependent Solver I** and choose **Fully Coupled**.
- 7 In the **Settings** window for **Fully Coupled**, locate the **General** section.
- 8 From the **Linear solver** list, choose **Direct**.
- 9 In the **Model Builder** window, click **Study 2 - Space Dependent**.
- 10 In the **Settings** window for **Study**, locate the **Study Settings** section.
- 11 Clear the **Generate default plots** check box.
- 12 In the **Study** toolbar, click  **Compute**.


RESULTS

Set up two **Sector 3D** datasets to rotate the 3D geometry according to its symmetry.

Sector 3D I


- 1 In the **Results** toolbar, click  **More Datasets** and choose **Sector 3D**.
- 2 In the **Settings** window for **Sector 3D**, locate the **Symmetry** section.
- 3 In the **Number of sectors** text field, type 4.
- 4 Click  **Plot**.
- 5 Right-click **Sector 3D I** and choose **Duplicate**.

Sector 3D 2




- 1 In the **Model Builder** window, click **Sector 3D 2**.
- 2 In the **Settings** window for **Sector 3D**, locate the **Symmetry** section.
- 3 From the **Sectors to include** list, choose **Manual**.
- 4 In the **Number of sectors to include** text field, type 3.
- 5 In the **Start sector** text field, type 3.
- 6 Click  **Plot**.

The following step creates Figures 3-6.

Bulk concentration B, 5 s

- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Bulk concentration B, 5 s in the **Label** text field.
- 3 Locate the **Data** section. From the **Time (s)** list, choose **5**.

Surface 1

- 1 Right-click **Bulk concentration B, 5 s** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Sector 3D 1**.
- 4 From the **Time (s)** list, choose **5**.
- 5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)>Transport of Diluted Species>Species cB>cB - Concentration - mol/m³**.
- 6 Click the  **Show Grid** button in the **Graphics** toolbar.
- 7 In the **Bulk concentration B, 5 s** toolbar, click  **Plot**.
- 8 Click the  **Zoom Extents** button in the **Graphics** toolbar.



Bulk concentration B, 5 s

In the **Model Builder** window, right-click **Bulk concentration B, 5 s** and choose **Duplicate**.

Bulk concentration B, 30 s

- 1 In the **Model Builder** window, under **Results** click **Bulk concentration B, 5 s 1**.
- 2 In the **Settings** window for **3D Plot Group**, type Bulk concentration B, 30 s in the **Label** text field.
- 3 Locate the **Data** section. From the **Time (s)** list, choose **30**.

Surface I

- 1 In the **Model Builder** window, expand the **Bulk concentration B, 30 s** node, then click **Surface I**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Sector 3D 2**.
- 4 From the **Time (s)** list, choose **30**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 6 In the **Bulk concentration B, 30 s** toolbar, click  **Plot**.




Bulk concentration B, 30 s

In the **Model Builder** window, right-click **Bulk concentration B, 30 s** and choose **Duplicate**.

Surface concentration B, 5 s

- 1 In the **Model Builder** window, under **Results** click **Bulk concentration B, 30 s I**.
- 2 In the **Settings** window for **3D Plot Group**, type Surface concentration B, 5 s in the **Label** text field.
- 3 Locate the **Data** section. From the **Time (s)** list, choose **5**.

Surface I

- 1 In the **Model Builder** window, expand the **Surface concentration B, 5 s** node, then click **Surface I**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Sector 3D 1**.
- 4 From the **Time (s)** list, choose **5**.
- 5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)>Surface Reactions 1>Surface species cs_B>cs_B - Surface concentration - mol/m²**.
- 6 Click the  **Transparency** button in the **Graphics** toolbar.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 8 In the **Surface concentration B, 5 s** toolbar, click  **Plot**.

Surface concentration B, 5 s




In the **Model Builder** window, right-click **Surface concentration B, 5 s** and choose **Duplicate**.

Surface concentration B, 30 s

- 1 In the **Model Builder** window, under **Results** click **Surface concentration B, 5 s I**.


- 2 In the **Settings** window for **3D Plot Group**, type Surface concentration B, 30 s in the **Label** text field.
- 3 Locate the **Data** section. From the **Time (s)** list, choose **30**.

Surface I

- 1 In the **Model Builder** window, expand the **Surface concentration B, 30 s** node, then click **Surface I**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Sector 3D 2**.
- 4 From the **Time (s)** list, choose **30**.
- 5 Click the  **Transparency** button in the **Graphics** toolbar.
- 6 Click the  **Zoom Extents** button in the **Graphics** toolbar.
- 7 In the **Surface concentration B, 30 s** toolbar, click  **Plot**.

Velocity field

Last, create [Figure 7](#) to visualize the velocity field within the 3D geometry.

- 1 In the **Home** toolbar, click  **Add Plot Group** and choose **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Velocity field in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **Custom**.
- 4 Find the **Type and data** subsection. Clear the **Type** check box.
- 5 Clear the **Description** check box.
- 6 Clear the **Unit** check box.
- 7 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.
- 8 Locate the **Color Legend** section. Select the **Show units** check box.

Streamline I

- 1 Right-click **Velocity field** and choose **Streamline**.
- 2 In the **Settings** window for **Streamline**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)>Laminar Flow I>Velocity and pressure>u,v,w - Velocity field**.
- 3 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Magnitude controlled**.
- 4 In the **Minimum distance** text field, type 0.03.
- 5 In the **Maximum distance** text field, type 0.05.

- 6 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.
- 7 Find the **Line style** subsection. From the **Type** list, choose **Tube**.


Color Expression /

- 1 Right-click **Streamline 1** and choose **Color Expression**.
- 2 In the **Settings** window for **Color Expression**, click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 2 (comp2)> Laminar Flow 1>Velocity and pressure>spf.U - Velocity magnitude - m/s**.

Surface /

- 1 In the **Model Builder** window, right-click **Velocity field** and choose **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Coloring and Style** section.
- 3 From the **Coloring** list, choose **Gradient**.
- 4 From the **Top color** list, choose **Custom**.
- 5 Click **Define custom colors**.
- 6 Set the RGB values to 166, 214, and 208, respectively.
- 7 Click **Add to custom colors**.
- 8 Click **Show color palette only** or **OK** on the cross-platform desktop.
- 9 From the **Bottom color** list, choose **Custom**.
- 10 Click **Define custom colors**.
- 11 Set the RGB values to 255, 160, and 122, respectively.
- 12 Click **Add to custom colors**.
- 13 Click **Show color palette only** or **OK** on the cross-platform desktop.


Selection /

- 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 **Walls**.
- 4 In the **Velocity field** toolbar, click  **Plot**.

Appendix — Geometry Modeling Instructions

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

NEW

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

ADD COMPONENT


In the **Home** toolbar, click  **Add Component** and choose **3D**.

GEOMETRY I

1 In the **Settings** window for **Geometry**, locate the **Units** section.

2 From the **Length unit** list, choose **mm**.

Cylinder I (cylI)

1 In the **Geometry** toolbar, click  **Cylinder**.

2 In the **Settings** window for **Cylinder**, locate the **Size and Shape** section.

3 In the **Radius** text field, type 4.25.

4 In the **Height** text field, type 2.15.

Block I (blkI)

1 In the **Geometry** toolbar, click  **Block**.

2 In the **Settings** window for **Block**, locate the **Size and Shape** section.

3 In the **Width** text field, type 4.25.

4 In the **Depth** text field, type 4.25.

5 In the **Height** text field, type 2.15.

Intersection I (intI)

1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Intersection**.

2 Click in the **Graphics** window and then press Ctrl+A to select both objects.

Sphere I (sphI)

1 In the **Geometry** toolbar, click  **Sphere**.

2 In the **Settings** window for **Sphere**, locate the **Size** section.

3 In the **Radius** text field, type 0.5.


4 Locate the **Position** section. In the **x** text field, type 0.45.

5 In the **y** text field, type 0.45.



6 In the **z** text field, type 0.45.

Array I (arrI)


1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.

- 2 Select the object **sph1** only.
- 3 In the **Settings** window for **Array**, locate the **Size** section.
- 4 In the **x size** text field, type 4.
- 5 In the **y size** text field, type 4.
- 6 In the **z size** text field, type 2.
- 7 Locate the **Displacement** section. In the **x** text field, type 0.95.
- 8 In the **y** text field, type 0.95.
- 9 In the **z** text field, type 0.95.
- 10 Locate the **Selections of Resulting Entities** section. Select the **Resulting objects selection** check box.
- 11 From the **Show in physics** list, choose **Boundary selection**.
- 12 Click  **Build Selected**.

Delete Entities I (del1)

- 1 In the **Geometry** toolbar, click  **Delete**.
- 2 Click the  **Wireframe Rendering** button in the **Graphics** toolbar.
- 3 Select the objects **arr1(3,4,1)**, **arr1(3,4,2)**, **arr1(4,3,1)**, **arr1(4,3,2)**, **arr1(4,4,1)**, and **arr1(4,4,2)** only.


Difference I (dif1)

- 1 In the **Geometry** toolbar, click  **Booleans and Partitions** and choose **Difference**.
- 2 Select the object **int1** only.
- 3 In the **Settings** window for **Difference**, locate the **Difference** section.
- 4 From the **Objects to subtract** list, choose **Array 1**.


Form Union (fin)

- 1 In the **Model Builder** window, click **Form Union (fin)**.
- 2 In the **Settings** window for **Form Union/Assembly**, click  **Build Selected**.


Column wall

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, locate the **Entities to Select** section.
- 3 From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 37 only.
- 5 In the **Label** text field, type Column wall.


Inlet

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Inlet in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 4 only.

Outlet column section

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Outlet column section in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundary 3 only.

Symmetry

- 1 In the **Geometry** toolbar, click  **Selections** and choose **Explicit Selection**.
- 2 In the **Settings** window for **Explicit Selection**, type Symmetry in the **Label** text field.
- 3 Locate the **Entities to Select** section. From the **Geometric entity level** list, choose **Boundary**.
- 4 On the object **fin**, select Boundaries 1 and 2 only.