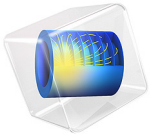

Protein Adsorption

This application simulates an ion-exchange column for protein adsorption. The fluid phase contains four components: two proteins, 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.

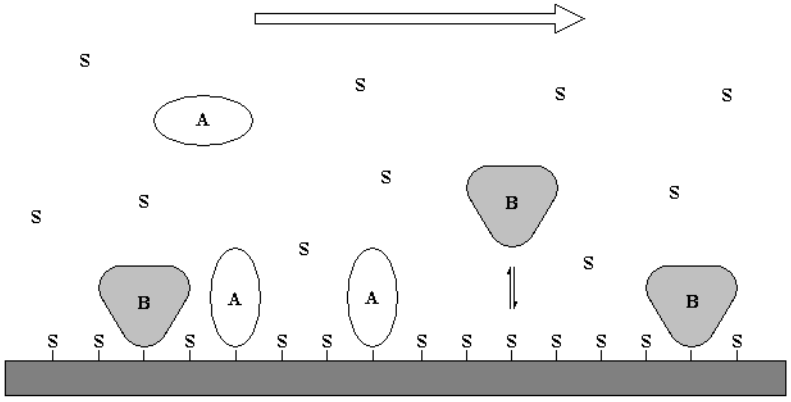

Figure 1: Proteins A and B displacing salt ions S at an ion-exchanger surface.

The equilibrium describing the adsorption/desorption reactions is

$$S(ads)+P \Leftrightarrow P(ads)+S \quad (1)$$

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.

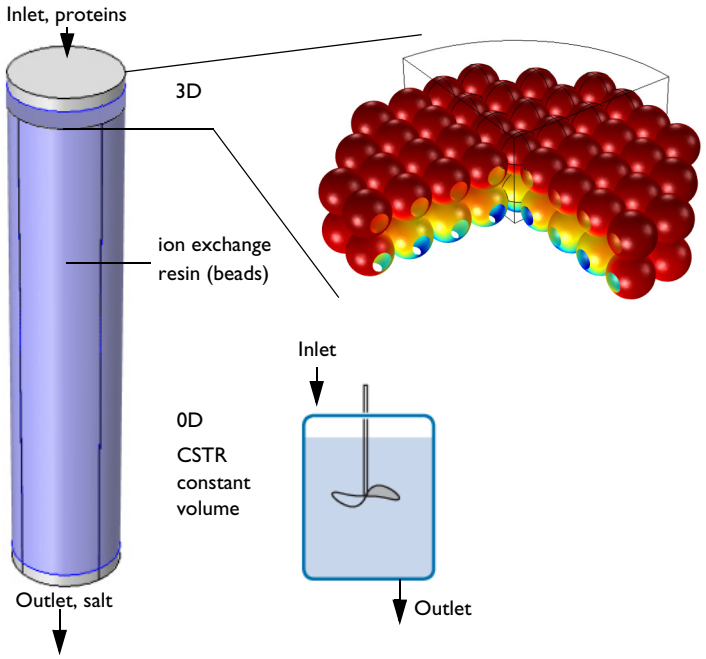

Figure 2: Ion-exchange column and model geometries. The 0D model approximates the entire column, while the 3D geometry is a detailed representation of a section at the top of the column.

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 $K_1^{\mathrm{eq}} = 2$ and for reaction 2, adsorption of B, is $K_2^{\mathrm{eq}} = 5$. These are entered as well, relating the concentrations as followed

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

$$K_2^{\mathrm{eq}} = \frac{c_S c_{B(\mathrm{ads})}}{c_B c_{S(\mathrm{ads})}} \tag{3}$$

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 $0.05\ \mathrm{mol/m^3}$. 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, i.e. 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 $0.05\ \mathrm{mol/m^3}$. In the column initially, the pores (the bulk) is filled with solvent and the ion-exchange beads are saturated with adsorbed salt.

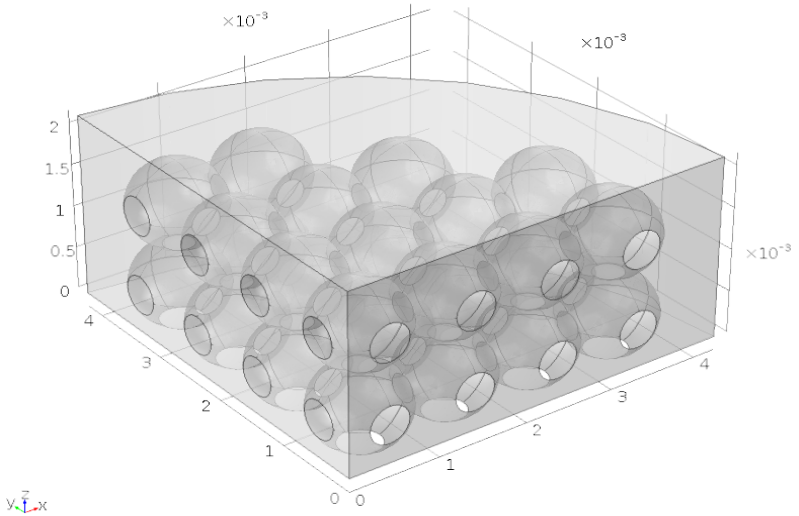

Figure 3: 3D model geometry.

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

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

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, i.e. 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.

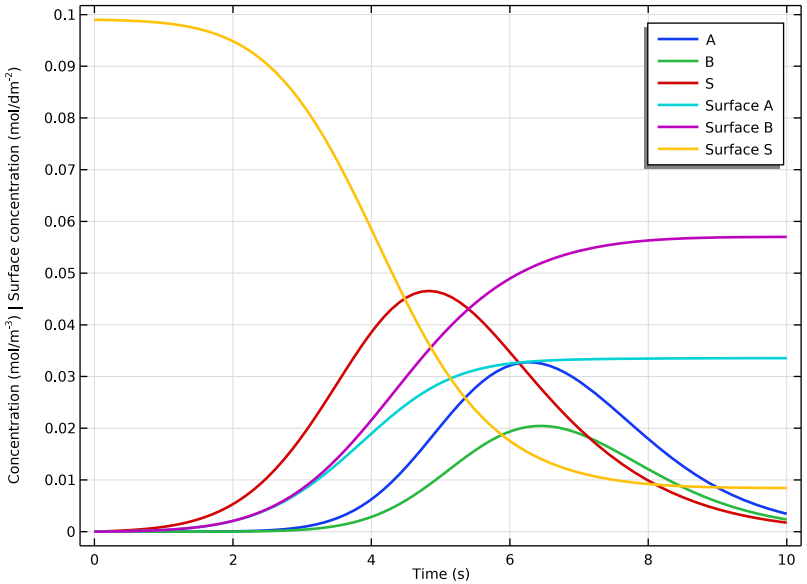

Figure 4: Concentrations of the reacting species as functions of time (s).

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.

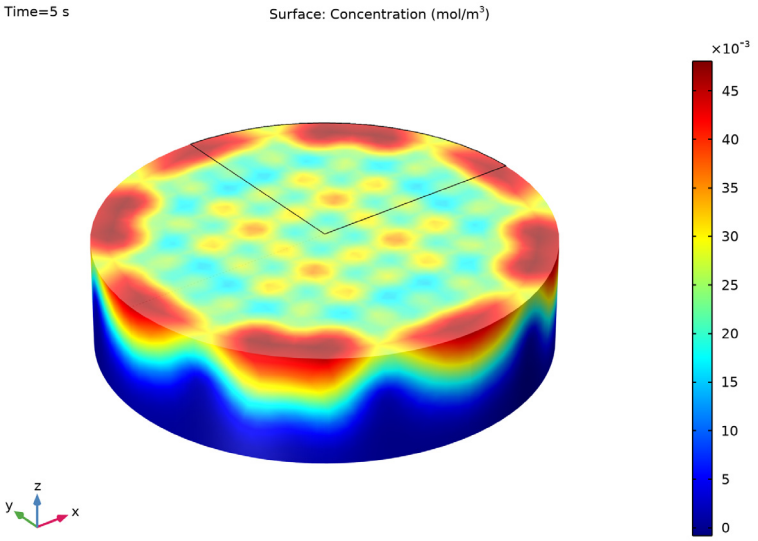

Figure 5: Bulk concentration of B at 5 s.

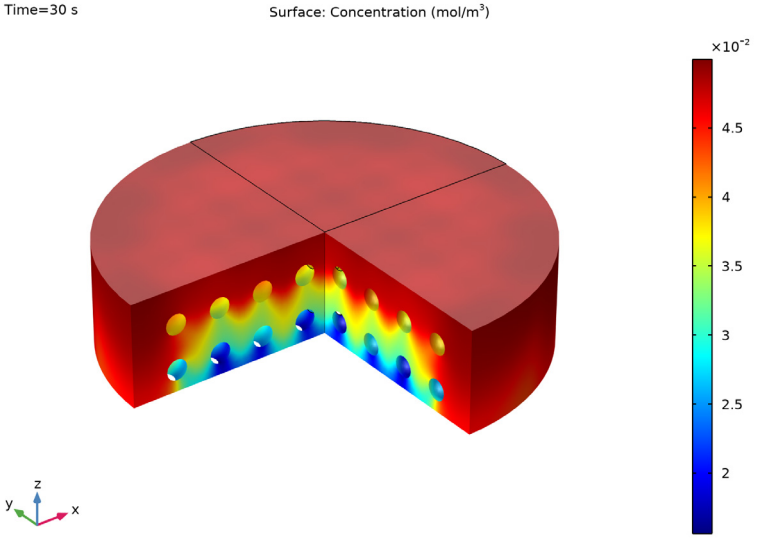

Figure 6: Bulk concentration of B at 30 s.

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/m^2).

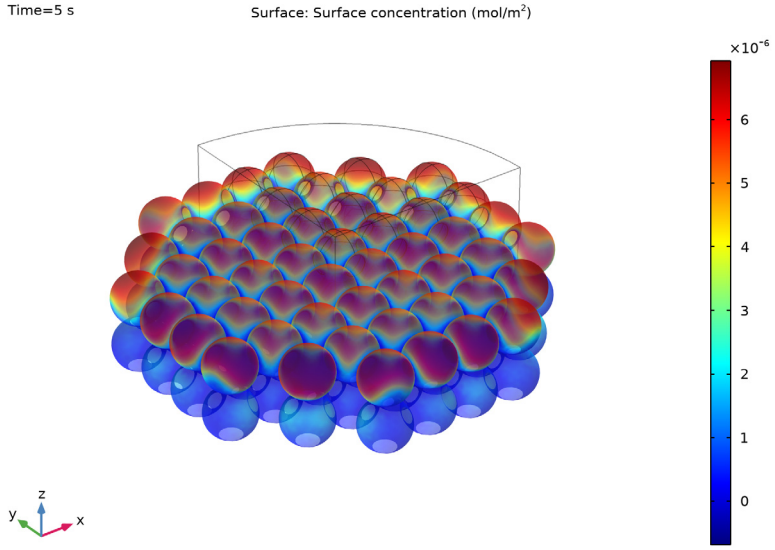

Figure 7: Surface concentration of B at 5 s.

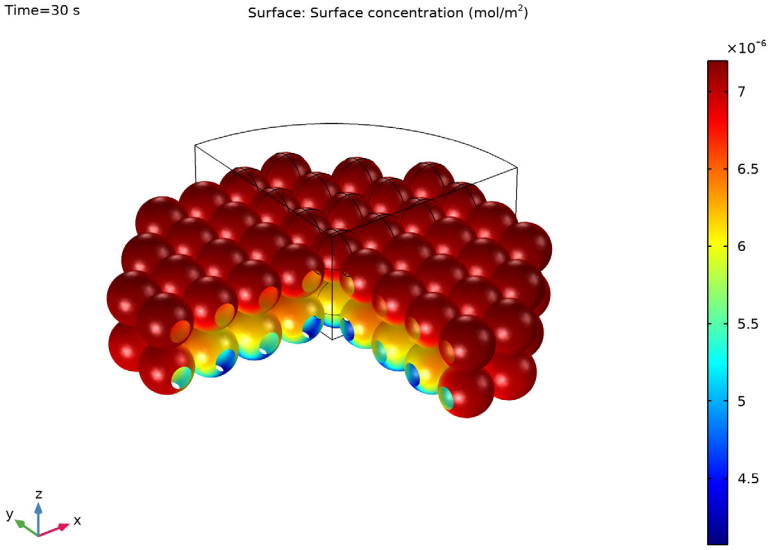

Figure 8: Surface concentration of B at 30 s.

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.

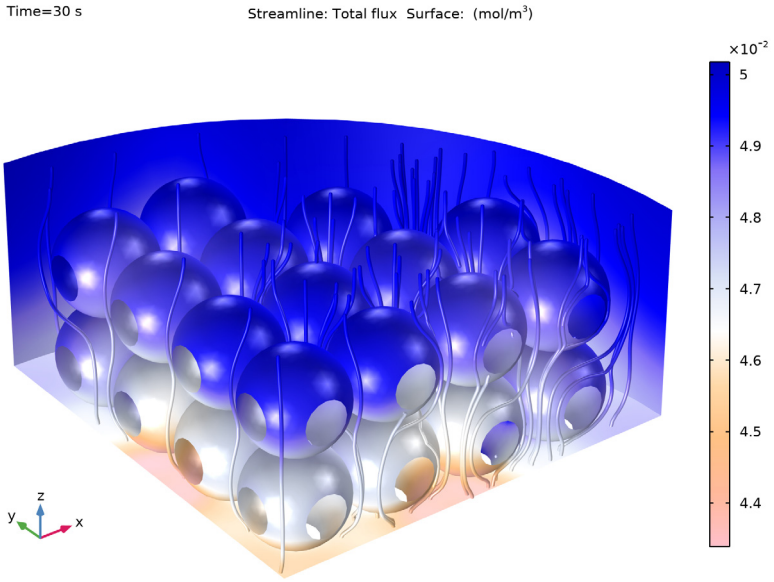

Figure 9: Velocity field in the pores of the column section.

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 **0D**.

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 1

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

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 1 (gp1)

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 1

1 In the **Model Builder** window, under **Component 1 (comp1)** 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_{eq0} text field, type `Keq01`.

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 `S(ads)+B=S+B(ads)`.

4 Click **Apply**.

5 Locate the **Equilibrium Settings** section. In the K_{eq0} text field, type `Keq02`.

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

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

7 In the **Settings** window for **Reaction Engineering**, click to expand the **Equilibrium Species Vector** section.

8 In the **Predefined dependent species (separated by ':')** text field, type `A(ads):B(ads)`.

9 Locate the **Reactor** section. Find the **Mass balance** subsection. From the **Volumetric rate** list, choose **User defined**.

Set `vp=0`, to neglect the volumetric production rate.

10 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.

11 Find the **Surface reaction area** subsection. In the A_r text field, type `Arsurf`.

Initial Values 1

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 1**.

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 (1)
S(ads)	`CS0surf`	1

Feed Inlet 1

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 `vfp`.

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

Species	Concentration (mol/m^3)
A	`CAmax_inlet*pulse11`
B	`CBmax_inlet*pulse11`

Enter densities and molar masses in the bulk species nodes.

Species: A

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MA.

4 In the ρ text field, type rho_p.

Species: S

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MS.

4 In the ρ text field, type rho_S.

Species: B

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MB.

4 In the ρ text field, type rho_p.

Enter also molar mass in the surface species nodes.

Surface species: S(ads)

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MS.

Surface species: A(ads)

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MA.

Surface species: B(ads)

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

2 In the **Settings** window for **Species**, locate the **General Parameters** section.

3 In the M text field, type MB.

Solve the 0D model for 10 s.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, under **Study 1** 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(0,0.1,10)`.

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 **1D 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.

5 In the associated text field, type `Concentration (mol/m<sup>-3</sup>) | Surface concentration (mol/dm<sup>-2</sup>)`.

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 1 (comp1)> 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 1 (comp1)>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 1 (comp1)>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 1 (comp1)>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 1 (comp1)>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 1 (comp1)>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. In the **Width** text field, type 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
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 1

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

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

3 In the text field, type H2O.

4 Locate the **Species Type** section. From the list, choose **Solvent**.

5 Locate the **General Parameters** section. In the M text field, type MH2O.

6 In the ρ text field, type rho_H2O.

Initial Values 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

For a liquid system with solvent, several transport parameters can be computed within the **Chemistry** interface. Activate this functionality by following these steps.

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 `myH2O`.

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

Generate Space-Dependent Model 1

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**.

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 1

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.

Inflow 1

1 In the **Model Builder** window, expand the **Component 2 (comp2)> Transport of Diluted Species (tds)** node, then 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 $c_{0,\mathrm{cA}}$ text field, type `CAmax_inlet`.

5 In the $c_{0,\mathrm{cB}}$ text field, type `CBmax_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**.

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, click **Initial Values 1**.

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

3 In the cA text field, type `CAmax_inlet*0.01`.

4 In the cB text field, type `CBmax_inlet*0.01`.

5 In the cS text field, type `1e-7`.

SURFACE REACTIONS 1 (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 1 (sr)**.

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

3 From the **Selection** list, choose **Array 1**.

Reactions 1

1 In the **Model Builder** window, expand the **Surface Reactions 1 (sr)** node, then click **Reactions 1**.

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 1

1 In the **Model Builder** window, click **Initial Values 1**.

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

3 In the cs_{A} text field, type `CS0surf*0.01`.

4 In the cs_{B} text field, type `CS0surf*0.01`.

LAMINAR FLOW 1 (SPF)

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

Inlet 1

1 In the **Model Builder** window, under **Component 2 (comp2)>Laminar Flow 1 (spf)** click **Inlet 1**.

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 1

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

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 1

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**.

MULTIPHYSICS

Reacting Flow, Diluted Species 1 (rfd1)

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

MESH 1

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

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 **Array 1**.

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 `9E-2`.

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 **All 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 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 `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

Stationary

1 In the **Study** toolbar, click  **Study Steps** and choose **Stationary>Stationary**.

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

3 In the table, clear the **Solve for** check boxes for **Reaction Engineering (re)**, **Chemistry 1 (chem)**, **Transport of Diluted Species (tds)**, and **Surface Reactions 1 (sr)**.

Step 1: Time Dependent

1 In the **Model Builder** window, 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(0,1,30)`.

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 1 (spf)**.

Step 2: Stationary

In the **Model Builder** window, under **Study 2** right-click **Step 2: Stationary** 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 1**.

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 **Time-Dependent Solver 1** 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**.

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

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

Sector 3D 1

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**.

Sector 3D 2

1 Right-click **Sector 3D 1** and choose **Duplicate**.

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

1 In the **Results** toolbar, click **3D Plot Group**.

2 In the **Settings** window for **3D Plot Group**, type `Bulk concentration B` in the **Label** text field.

Surface 1

1 Right-click **Bulk concentration B** 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.

Bulk concentration B

1 In the **Model Builder** window, click **Bulk concentration B**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **5**.

4 In the **Bulk concentration B** toolbar, click **Plot**.

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

Surface 1

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

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**.

Bulk concentration B

1 In the **Model Builder** window, click **Bulk concentration B**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **30**.

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

5 In the **Bulk concentration B** toolbar, click  **Plot**.

Surface concentration B

1 Right-click **Bulk concentration B** and choose **Duplicate**.

2 In the **Settings** window for **3D Plot Group**, type `Surface concentration B` in the **Label** text field.

Surface 1

1 In the **Model Builder** window, expand the **Surface concentration B** node, then click **Surface 1**.

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**.

Surface concentration B

1 In the **Model Builder** window, click **Surface concentration B**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **5**.

4 Click the  **Transparency** button in the **Graphics** toolbar.

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

6 In the **Surface concentration B** toolbar, click  **Plot**.

Surface 1

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

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**.

Surface concentration B

1 In the **Model Builder** window, click **Surface concentration B**.

2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.

3 From the **Time (s)** list, choose **30**.

4 Click the **Transparency** button in the **Graphics** toolbar.

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

6 In the **Surface concentration B** 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 Locate the **Plot Settings** section. Clear the **Plot dataset edges** check box.

Streamline 1

1 Right-click **Velocity field** and choose **Streamline**.

2 In the **Settings** window for **Streamline**, locate the **Streamline Positioning** section.

3 From the **Positioning** list, choose **Magnitude controlled**.

4 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.

Color Expression 1

1 Right-click **Streamline 1** and choose **Color Expression**.

2 In the **Settings** window for **Color Expression**, locate the **Coloring and Style** section.

3 From the **Color table** list, choose **Twilight**.

Surface 1

1 In the **Model Builder** window, right-click **Velocity field** and choose **Surface**.

2 In the **Settings** window for **Surface**, click to expand the **Inherit Style** section.

3 From the **Plot** list, choose **Streamline 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 **All boundaries**.

4 In the list, select **1**.

5 Click — **Remove from Selection**.

6 Select Boundaries 2–213 only.

7 In the list, select **2**.

8 Click — **Remove from Selection**.

9 Select Boundaries 3–213 only.

10 In the list, select **4**.

11 Click — **Remove from Selection**.

12 Select Boundaries 3 and 5–213 only.

13 In the **Velocity field** toolbar, click  **Plot**.

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