



Model created in COMSOL Multiphysics 6.4

# Liquid-Liquid Extraction

## *Introduction*

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Liquid–liquid extraction is a process used to separate or transfer species between two immiscible liquids. Transfer of species from one phase to the other is driven by a difference in relative solubility. Often in mixtures consisting of two different phases, one phase disperses within the other phase. This phase is referred to as the dispersed phase, while the other phase is referred to as the continuous phase. Which phase becomes the dispersed phase depends on the density of the two phases.

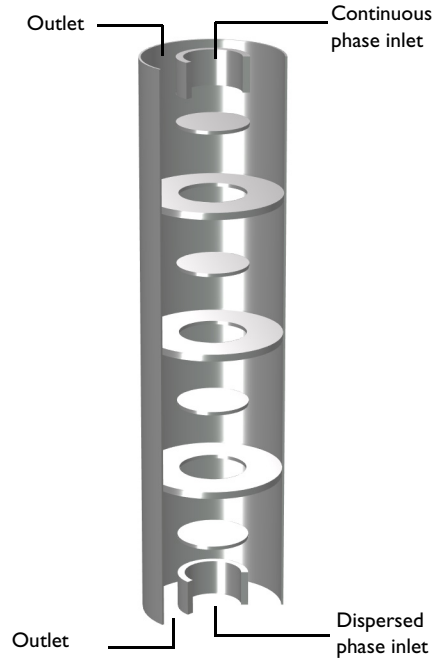
In this example, a water-filled extraction column is studied. Oil, containing a solute species, is injected at the bottom of the column and rises up due to buoyancy. The raffinate exits at the top of the column. As the oil droplets rise, the solute species is transferred to the solvent, the water phase. Water is initially in the column and is continuously injected at the top. The extract exits at the bottom of the column. In this setup, the water phase becomes the continuous phase and the oil forms droplets as the dispersed phase. The column is fitted with a number of alternating horizontal discs in order to increase the residence time of the oil droplets.

## *Model Definition*

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The extraction is modeled using the Dispersed Two-Phase Flow, Diluted Species multiphysics interface, where the  $k$ – $\omega$  model is used to account for the turbulent flow from the rising droplets. The species transport is solved for in both the continuous (water) phase and in the dispersed phase (oil droplets).

The extraction column can be constructed using a 2D axisymmetric geometry due to rotational symmetry. The column is 0.8 m tall with a radius of 0.1 m. At each end, a wall separates an inflow and outflow. Alternating inner and outer horizontal discs are located throughout the column with a spacing of 0.1 m, as seen in [Figure 1](#). The inner discs have a radius of 0.5 m. The outer disc openings also have a radius of 0.5 m.



*Figure 1: Geometry of the modeled extraction column.*

Water enters the extraction column at the top inlet and oil enters at the bottom inlet with an oil volume fraction of 0.5. No species is present in the ingoing water. The oil phase enters with a solute species concentration of  $10 \text{ mol/m}^3$ . The water phase at the top inlet has an inlet velocity of  $0.01 \text{ m/s}$ . The water phase flows from the top to the bottom of the column due to gravity. The density difference between the oil droplets and surrounding water induces buoyancy, causing the droplets to rise through the column.

A pressure condition is used at the outlets. The relative pressure is specified as  $0 \text{ Pa}$  at the bottom outlet. At the top outlet the relative pressure is specified as

$$P_0 = -g\rho z \quad (1)$$

where  $g$  is the gravitational acceleration ( $\text{m/s}^2$ ),  $\rho$  is the mixture density ( $\text{kg/m}^3$ ), and  $z$  the height above the column bottom. The flow is solved for by the Mixture Model using the  $k$ - $\omega$  turbulence model.

## MASS TRANSPORT

The rate of solute extraction,  $R_e$  (mol/m<sup>3</sup>/s), from the dispersed phase to the continuous phase is modeled according to

$$R_e = -k_m(K_p c_c - c_d)a_s \quad (2)$$

where  $k_m$  is the mass transfer coefficient (m/s);  $K_p$  the partition coefficient;  $c_c$  and  $c_d$  the species concentrations in the continuous and dispersed phases (mol/m<sup>3</sup>), respectively; and  $a_s$  is the specific surface area of the oil droplets per unit volume (1/m). The partition coefficient describes the distribution of solute between the two phases at equilibrium. The specific surface area of the droplets is calculated as

$$a_s = \frac{3\phi_d}{r_p} \quad (3)$$

where the droplets are assumed to be spherical. In this equation,  $\phi_d$  is the dispersed phase volume fraction and  $r_p$  is the droplet radius. Including convective and diffusive transport, the time-dependent solute mass transport in the continuous and dispersed phases is modeled according to

$$\frac{\partial c_c}{\partial t} + \nabla \cdot (-D\nabla c_c + \mathbf{u}c_c) = R_e \quad (4)$$

and

$$\frac{\partial c_d}{\partial t} + \nabla \cdot (-D\nabla c_d + \mathbf{u}c_d) = -R_e \quad (5)$$

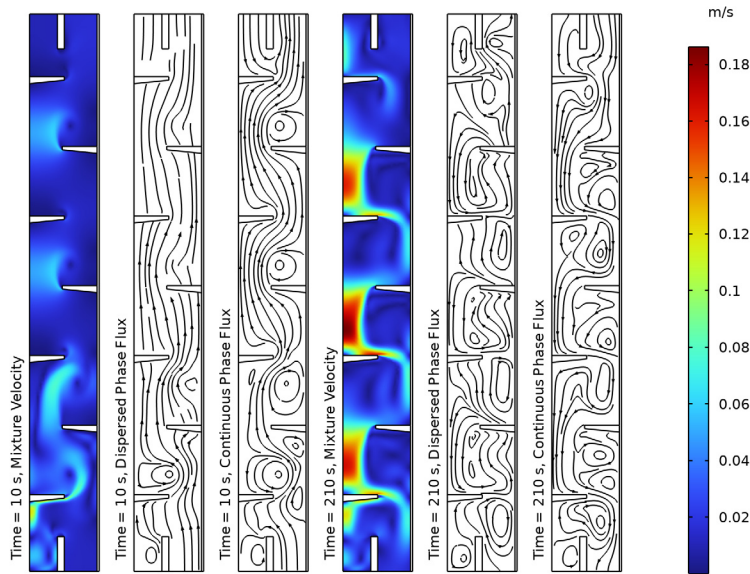
Here,  $D$  is the diffusion coefficient (m<sup>2</sup>/s) and the vector  $\mathbf{u}$  is the velocity field (m/s). The diffusivity coefficient is the sum of the fluid diffusion and the turbulent diffusion from the multiphysics coupling. The turbulent diffusivity is calculated from the turbulent kinematic viscosity,  $\nu_t$  (m<sup>2</sup>/s) and the turbulent Schmidt number,  $Sc_T$ , as

$$D_T = \frac{\nu_t}{Sc_T} \quad (6)$$

To account for the area between the wall and the developed turbulent flow, mass transport wall functions are also modeled using the Dispersed Two-Phase Flow, Diluted Species multiphysics coupling interface.

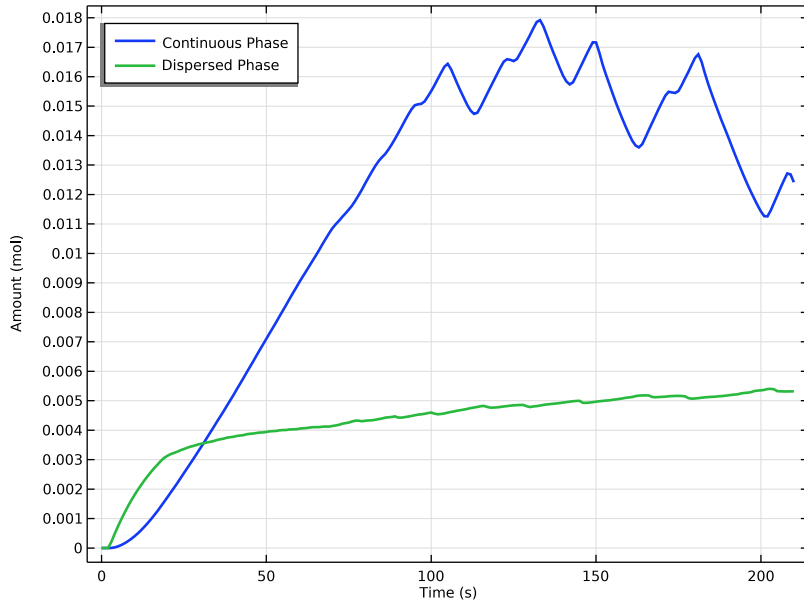
## Results and Discussion

The 2D mixture velocity and phase fluxes at 10 and 210 s is shown in [Figure 2](#). At 10 s the dispersed phase has begun entering the column and the highest mixture velocity can be seen at the oil inlet. At this point the column mainly contains water. The flux of the water phase can be seen from the continuous phase flux streamlines. At 210 s the dispersed phase flux has developed throughout the entire column.



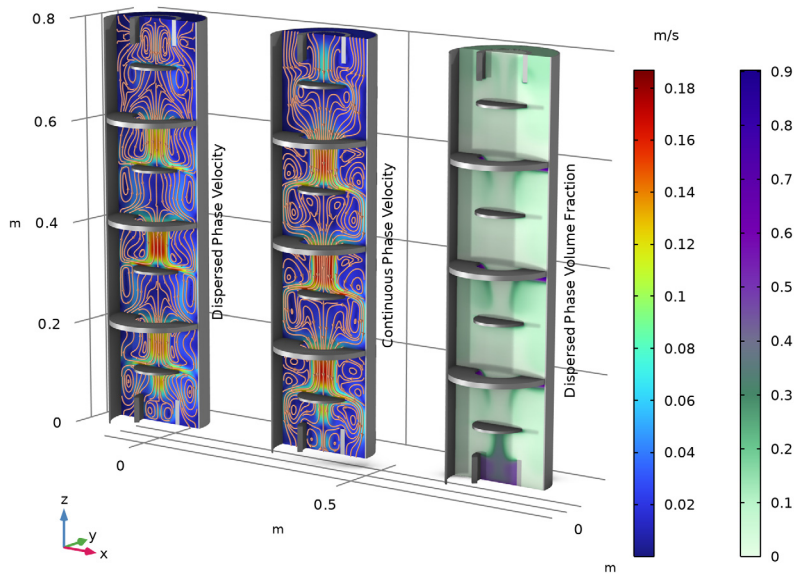
*Figure 2: Mixture velocity (m/s) and phase flux stream lines at 10 and 210 s.*

The total phase specific solute content is seen in [Figure 3](#). The solute species enters the column with the dispersed phase. As soon as the solute enters the column it begins transferring from the dispersed to the continuous phase. After about 30 s the amount of solute is larger in the continuous phase than in the dispersed phase.



*Figure 3: Total amount of solute species in the dispersed and continuous phase.*

Figure 4 shows the phase velocities and dispersed phase volume fraction after 210 s. The phase velocities increase when passing through the disc openings as the surface area decreases. The dispersed phase volume fraction is the largest on the bottom of the outer discs.



*Figure 4: Phase velocities and dispersed phase volume fraction at 210 s.*

The specific phase concentrations and extraction rate is seen in [Figure 5](#). The concentration is overall higher in the dispersed phase than the continuous phase due to the difference in volume. As shown in [Equation 2](#), the extraction rate is the highest where the concentration difference is the largest. This occurs at the bottom of the column, close to the oil inlet.

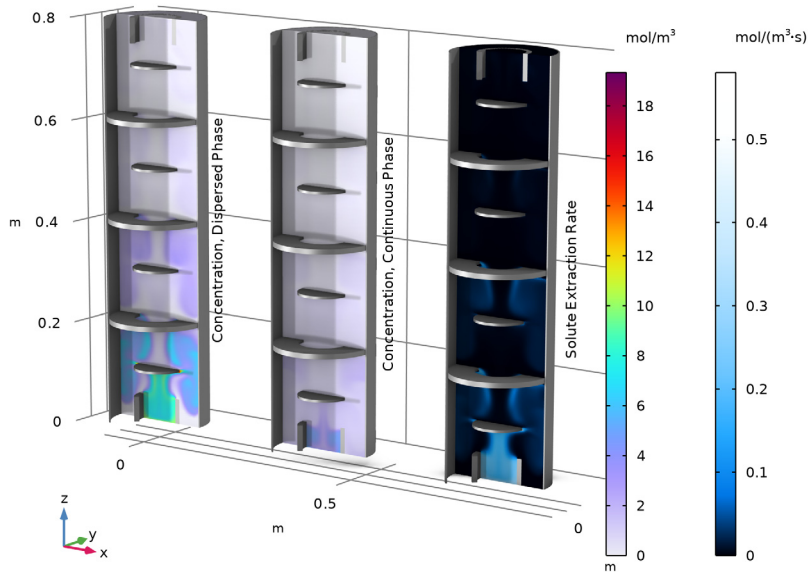


Figure 5: Phase specific species concentrations and extraction rate at 210 s.

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**Application Library path:** Chemical\_Reaction\_Engineering\_Module/  
Mixing\_and\_Separation/liquid\_liquid\_extraction


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### *Modeling Instructions*


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

#### **NEW**

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

#### **MODEL WIZARD**

- 1 In the **Model Wizard** window, click  **2D Axisymmetric**.
- 2 In the **Select Physics** tree, select **Chemical Species Transport > Dispersed Two-Phase Flow with Species Transport > Turbulent Flow > Turbulent Flow, k- $\omega$** .
- 3 Click **Add**.

- 4 In the **Added physics interfaces** tree, select **Continuous Phase Transport of Diluted Species (tds)**.
- 5 In the **Concentrations (mol/m<sup>3</sup>)** table, enter the following settings:

cc

- 6 In the **Added physics interfaces** tree, select **Dispersed Phase Transport of Diluted Species (tds2)**.
- 7 In the **Concentrations (mol/m<sup>3</sup>)** table, enter the following settings:


cd

- 8 Click  **Study**.
- 9 In the **Select Study** tree, select **General Studies > Time Dependent**.
- 10 Click  **Done**.

Import the parameters for the model.

## GLOBAL DEFINITIONS


### *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 `liquid_liquid_extraction_parameters.txt`.


## DEFINITIONS

Define step functions that will be used to smoothen sharp transitions in the model.


### *Step 1 (step1)*

- 1 In the **Definitions** toolbar, click  **More Functions** and choose **Step**.
- 2 In the **Settings** window for **Step**, locate the **Parameters** section.
- 3 In the **Location** text field, type 0.64.
- 4 In the **From** text field, type 1.
- 5 In the **To** text field, type 0.
- 6 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type 0.15.

### Step 2 (step2)


- 1 In the **Definitions** toolbar, click  **More Functions** and choose **Step**.
- 2 In the **Settings** window for **Step**, locate the **Parameters** section.
- 3 In the **Location** text field, type 0.5.
- 4 Locate the **Smoothing** section. In the **Size of transition zone** text field, type 1[s].

### Step 3 (step3)

- 1 In the **Definitions** toolbar, click  **More Functions** and choose **Step**.
- 2 In the **Settings** window for **Step**, locate the **Parameters** section.
- 3 In the **Location** text field, type 2.25.
- 4 Locate the **Smoothing** section. In the **Size of transition zone** text field, type 0.5[s].

## GEOMETRY I


### Rectangle 1 (r1)

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type R\_c.
- 4 In the **Height** text field, type H\_c.
- 5 Click to expand the **Layers** section. In the table, enter the following settings:

Layer name	Thickness (m)
Layer 1	t_c

- 6 Select the **Layers to the right** checkbox.
- 7 Clear the **Layers on bottom** checkbox.

### Rectangle 2 (r2)

- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type W\_sep.
- 4 In the **Height** text field, type H\_sep.
- 5 Locate the **Position** section. In the **r** text field, type R\_c\*0.4.


Mirror the geometry to cover the entire extraction column.

### Mirror 1 (mir1)

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


- 2 Select the object **r2** only.
- 3 In the **Settings** window for **Mirror**, locate the **Input** section.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Point on Line of Reflection** section. In the **z** text field, type  $H_c/2$ .
- 6 Locate the **Normal Vector to Line of Reflection** section. In the **r** text field, type 0.
- 7 In the **z** text field, type 1.

*Polygon 1 (poll)*


- 1 In the **Geometry** toolbar, click  **Polygon**.
- 2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.
- 3 In the table, enter the following settings:

<b>r (m)</b>	<b>z (m)</b>
0	h0_s
R_c/2	h0_s
R_c/2	h0_s-0.5 [cm]
0	h0_s-1 [cm]
0	h0_s


*Array 1 (arr1)*

- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Array**.
- 2 Select the object **poll** only.
- 3 In the **Settings** window for **Array**, locate the **Size** section.
- 4 In the **z size** text field, type n\_s.
- 5 Locate the **Displacement** section. In the **z** text field, type hsep\_s\*2.

*Mirror 2 (mir2)*


- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Mirror**.
- 2 Select the objects **arr1(1,1)**, **arr1(1,2)**, and **arr1(1,3)** only.
- 3 In the **Settings** window for **Mirror**, locate the **Input** section.
- 4 Select the **Keep input objects** checkbox.
- 5 Locate the **Point on Line of Reflection** section. In the **r** text field, type  $(R_c-t_c)/2$ .

*Move 1 (mov1)*



- 1 In the **Geometry** toolbar, click  **Transforms** and choose **Move**.
- 2 Select the objects **mir2(1)**, **mir2(2)**, and **mir2(3)** only.

- 3 In the **Settings** window for **Move**, locate the **Displacement** section.
- 4 In the **z** text field, type  $h_{sep\_s}$ .

#### *Rectangle 3 (r3)*


- 1 In the **Geometry** toolbar, click  **Rectangle**.
- 2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 3 In the **Width** text field, type  $R_c * 0.4 * 0.9$ .
- 4 In the **Height** text field, type  $h0\_s * 0.85$ .

#### *Mesh Control Domains 1 (mcd1)*

- 1 In the **Geometry** toolbar, click  **Virtual Operations** and choose **Mesh Control Domains**.
- 2 On the object **fin**, select Domain 1 only.
- 3 In the **Geometry** toolbar, click  **Build All**.

### DEFINITIONS


#### *Column interior*

- 1 In the **Definitions** toolbar, click  **Explicit**.
- 2 In the **Settings** window for **Explicit**, type *Column interior* in the **Label** text field.
- 3 Select Domain 1 only.



#### *Maximum 1 (maxo1)*

- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Maximum**.
- 2 Select Domain 1 only.

#### *Minimum 1 (minop1)*

- 1 In the **Definitions** toolbar, click  **Nonlocal Couplings** and choose **Minimum**.
- 2 In the **Settings** window for **Minimum**, locate the **Source Selection** section.
- 3 From the **Selection** list, choose **All domains**.

### 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 the **Add to Component** button in the window toolbar.
- 5 In the **Home** toolbar, click  **Add Material** to close the **Add Material** window.

## MIXTURE MODEL, K- $\omega$ (MM)

- 1 In the **Settings** window for **Mixture Model, k- $\omega$** , locate the **Domain Selection** section.
- 2 From the **Selection** list, choose **Column interior**.
- 3 Locate the **Physical Model** section. From the **Dispersed phase** list, choose **Liquid droplets/bubbles**.
- 4 From the **Slip model** list, choose **Schiller–Naumann**.


### *Mixture Properties 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Mixture Model, k- $\omega$  (mm)** click **Mixture Properties 1**.
- 2 In the **Settings** window for **Mixture Properties**, locate the **Materials** section.
- 3 From the **Dispersed phase** list, choose **Domain material**.
- 4 Locate the **Dispersed Phase Properties** section. From the  $\rho_d$  list, choose **User defined**. In the associated text field, type rho\_d.
- 5 From the  $\mu_d$  list, choose **User defined**. In the associated text field, type mu\_d.
- 6 In the  $d_d$  text field, type 2\*r\_d.
- 7 Locate the **Mixture Model** section. From the **Mixture viscosity model** list, choose **Volume averaged**.


### *Gravity 1*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Gravity**.
- 2 Select Domain 1 only.

### *Outlet 1*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outlet**.
- 2 Select Boundary 36 only.
- 3 In the **Settings** window for **Outlet**, locate the **Pressure** section.
- 4 Clear the **Suppress backflow** checkbox.
- 5 Locate the **Dispersed Phase Boundary Condition** section. Select the **Exterior dispersed phase conditions** checkbox.
- 6 In the  $\phi_{d,0}$  text field, type 1e-6.

### *Outlet 2*


- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Outlet**.
- 2 Select Boundary 42 only.
- 3 In the **Settings** window for **Outlet**, locate the **Pressure** section.

- 4 In the  $p_0$  text field, type `-g_const*mm.rho*z`.
- 5 Locate the **Dispersed Phase Boundary Condition** section. Select the **Exterior dispersed phase conditions** checkbox.
- 6 In the  $\phi_{d,0}$  text field, type `1e-6`.

#### *Inlet 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inlet**.
- 2 Select Boundary 2 only.
- 3 In the **Settings** window for **Inlet**, locate the **Velocity** section.
- 4 In the  $J_0$  text field, type `nojac(mm.jslipz)`.
- 5 Locate the **Dispersed Phase Boundary Condition** section. In the  $\phi_{d,0}$  text field, type `vf0*step2(t)`.

#### *Inlet 2*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inlet**.
- 2 Select Boundary 19 only.
- 3 In the **Settings** window for **Inlet**, locate the **Velocity** section.
- 4 In the  $J_0$  text field, type `0.01[m/s]*step2(t)`.

### **CONTINUOUS PHASE TRANSPORT OF DILUTED SPECIES (TDS)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Continuous Phase Transport of Diluted Species (tds)**.
- 2 In the **Settings** window for **Continuous Phase Transport of Diluted Species**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Column interior**.


#### *Fluid 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Continuous Phase Transport of Diluted Species (tds)** click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.
- 3 In the  $D_{cc}$  text field, type `D1`.

#### *Inflow 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.
- 2 Select Boundary 19 only.

#### *Open Boundary 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Open Boundary**.
- 2 Select Boundaries 2, 36, and 42 only.
- 3 In the **Settings** window for **Open Boundary**, locate the **Exterior Concentration** section.
- 4 In the  $c_{0,cc}$  text field, type  $1e-6$ .


#### **DISPERSED PHASE TRANSPORT OF DILUTED SPECIES 2 (TDS2)**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Dispersed Phase Transport of Diluted Species 2 (tds2)**.
- 2 In the **Settings** window for **Dispersed Phase Transport of Diluted Species**, locate the **Domain Selection** section.
- 3 From the **Selection** list, choose **Column interior**.


#### *Fluid 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Dispersed Phase Transport of Diluted Species 2 (tds2)** click **Fluid 1**.
- 2 In the **Settings** window for **Fluid**, locate the **Diffusion** section.
- 3 In the  $D_{cd}$  text field, type  $D1$ .

#### *Inflow 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Inflow**.
- 2 Select Boundary 2 only.
- 3 In the **Settings** window for **Inflow**, locate the **Concentration** section.
- 4 In the  $c_{0,cd}$  text field, type  $cd_0*vf0*step3(t)$ .

#### *Open Boundary 1*

- 1 In the **Physics** toolbar, click  **Boundaries** and choose **Open Boundary**.
- 2 Select Boundaries 19, 36, and 42 only.
- 3 In the **Settings** window for **Open Boundary**, locate the **Exterior Concentration** section.
- 4 In the  $c_{0,cd}$  text field, type  $1e-6$ .

#### **MULTIPHYSICS**

##### *Dispersed Two-Phase Flow, Diluted Species 1 (dds1)*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Multiphysics** click **Dispersed Two-Phase Flow, Diluted Species 1 (dds1)**.

- 2 In the **Settings** window for **Dispersed Two-Phase Flow, Diluted Species**, locate the **Solute Extraction** section.
- 3 Select the **Species cc** checkbox.
- 4 In the  $k_{m,cc}$  text field, type  $km*step1$  (phid).
- 5 In the  $K_{p,cc}$  text field, type  $K_p$ .

#### **MESH 1**

- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
- 2 In the **Settings** window for **Mesh**, locate the **Sequence Type** section.
- 3 From the list, choose **User-controlled mesh**.

#### *Size*

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Mesh 1** click **Size**.
- 2 In the **Settings** window for **Size**, locate the **Element Size** section.
- 3 From the **Predefined** list, choose **Coarse**.
- 4 Click the **Custom** button.
- 5 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type 0.005.
- 6 In the **Minimum element size** text field, type  $4.0E-5$ .
- 7 In the **Curvature factor** text field, type 0.25.

#### *Corner Refinement 1*

- 1 In the **Model Builder** window, click **Corner Refinement 1**.
- 2 In the **Settings** window for **Corner Refinement**, locate the **Angle** section.
- 3 In the **Minimum angle between boundaries** text field, type 200.
- 4 Locate the **Refinement** section. In the **Element size scaling factor** text field, type 0.2.

#### *Free Triangular 1*



- 1 In the **Model Builder** window, click **Free Triangular 1**.
- 2 In the **Settings** window for **Free Triangular**, locate the **Domain Selection** section.
- 3 From the **Geometric entity level** list, choose **Remaining**.

#### *Boundary Layers 1*

- 1 In the **Model Builder** window, click **Boundary Layers 1**.
- 2 In the **Settings** window for **Boundary Layers**, click to expand the **Corner Settings** section.
- 3 From the **Handling of sharp corners** list, choose **Splitting**.

- 4 In the **Maximum angle per split** text field, type 45.
- 5 Click to expand the **Transition** section. In the **Number of iterations** text field, type 10.

#### *Size 2*

- 1 In the **Mesh** toolbar, click  **Sizing** and choose **Size**.
- 2 In the **Settings** window for **Size**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domain 1 only.
- 5 Locate the **Element Size** section. From the **Calibrate for** list, choose **Fluid dynamics**.
- 6 From the **Predefined** list, choose **Finer**.
- 7 Drag and drop below **Size 1**.
- 8 Click  **Build All**.

#### **STUDY 1**


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

Change the time interval to see the startup process.

#### *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, 1, 210).

#### *Solution 1 (sol1)*

- 1 In the **Study** toolbar, click  **Show Default Solver**.
- 2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node.
- 3 In the **Model Builder** window, expand the **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** node, then click **Concentration (comp1.cd)**.
- 4 In the **Settings** window for **Field**, locate the **Scaling** section.
- 5 From the **Method** list, choose **Manual**.
- 6 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Concentration (comp1.cd)**.
- 7 In the **Settings** window for **Field**, locate the **Scaling** section.
- 8 From the **Method** list, choose **Manual**.

- 9 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Wall Concentration, Downside (comp1.dds1.cWall\_d\_cc)**.
- 10 In the **Settings** window for **Field**, locate the **Scaling** section.
- 11 From the **Method** list, choose **Manual**.
- 12 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Wall Concentration, Downside (comp1.dds1.cWall\_d\_cd)**.
- 13 In the **Settings** window for **Field**, locate the **Scaling** section.
- 14 From the **Method** list, choose **Manual**.
- 15 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Wall Concentration, Upside (comp1.dds1.cWall\_u\_cc)**.
- 16 In the **Settings** window for **Field**, locate the **Scaling** section.
- 17 From the **Method** list, choose **Manual**.
- 18 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Wall Concentration, Upside (comp1.dds1.cWall\_u\_cd)**.
- 19 In the **Settings** window for **Field**, locate the **Scaling** section.
- 20 From the **Method** list, choose **Manual**.
- 21 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Velocity Field, Mixture (comp1.j)**.
- 22 In the **Settings** window for **Field**, locate the **Scaling** section.
- 23 From the **Method** list, choose **Manual**.
- 24 In the **Scale** text field, type 0.1.
- 25 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1) > Dependent Variables 1** click **Pressure (comp1.p)**.
- 26 In the **Settings** window for **Field**, locate the **Scaling** section.
- 27 From the **Method** list, choose **Manual**.
- 28 In the **Scale** text field, type  $1e4$ .  
Modify the maximum step constraint.
- 29 In the **Model Builder** window, under **Study 1 > Solver Configurations > Solution 1 (sol1)** click **Time-Dependent Solver 1**.
- 30 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 31 From the **Maximum step constraint** list, choose **Constant**.
- 32 In the **Maximum step** text field, type  $5e-3$ .

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

## RESULTS


### *Revolution 2D 1*

- 1 In the **Model Builder** window, expand the **Results** node.
- 2 Right-click **Results** > **Datasets** and choose **Revolution 2D**.
- 3 In the **Settings** window for **Revolution 2D**, click to expand the **Revolution Layers** section.
- 4 In the **Revolution angle** text field, type 180.


### *Revolution 2D 2*

In the **Results** toolbar, click  **More Datasets** and choose **Revolution 2D**.


### *Selection*

- 1 In the **Results** toolbar, click  **Attributes** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domains 2–5 and 8–10 only.


### *Revolution 2D 3*

- 1 In the **Results** toolbar, click  **More Datasets** and choose **Revolution 2D**.
- 2 In the **Settings** window for **Revolution 2D**, locate the **Revolution Layers** section.
- 3 In the **Revolution angle** text field, type 225.

### *Selection*


- 1 In the **Results** toolbar, click  **Attributes** and choose **Selection**.
- 2 In the **Settings** window for **Selection**, locate the **Geometric Entity Selection** section.
- 3 From the **Geometric entity level** list, choose **Domain**.
- 4 Select Domains 6, 7, and 11 only.

### *Cut Plane 1*

- 1 In the **Results** toolbar, click  **Cut Plane**.
- 2 In the **Settings** window for **Cut Plane**, locate the **Plane Data** section.
- 3 From the **Plane** list, choose **xz-planes**.


Now, show the mixture velocity and the phase fluxes with streamlines.

### *Mixture Velocity and Phase Flux Streamlines*

- 1 In the **Results** toolbar, click  **2D Plot Group**.

- 2 In the **Settings** window for **2D Plot Group**, type Mixture Velocity and Phase Flux Streamlines in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 4 Click to expand the **Color Legend** section. Select the **Show units** checkbox.
- 5 Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.
- 6 In the **Relative padding** text field, type 0.5.

#### *Mixture Velocity*

- 1 In the **Mixture Velocity and Phase Flux Streamlines** toolbar, click  **Surface**.
- 2 In the **Settings** window for **Surface**, type Mixture Velocity in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.
- 4 From the **Time (s)** list, choose **10**.
- 5 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Velocity and pressure > mm.J - Velocity field, mixture - m/s**.

#### *Mixture Velocity and Phase Flux Streamlines*

In the **Mixture Velocity and Phase Flux Streamlines** toolbar, click  **Streamline**.

#### *Phase Flux, Dispersed Phase*

- 1 In the **Settings** window for **Streamline**, type Phase Flux, Dispersed Phase in the **Label** text field.
- 2 Locate the **Data** section. From the **Dataset** list, choose **Study 1/Solution 1 (sol1)**.
- 3 From the **Time (s)** list, choose **10**.
- 4 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Fluxes > mm.jdr,mm.jdz - Dispersed phase flux**.
- 5 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.
- 6 In the **Density level** text field, type 7.8.
- 7 Locate the **Coloring and Style** section. Find the **Point style** subsection. From the **Type** list, choose **Arrow**.

#### *Phase Flux, Continuous Phase*

- 1 Right-click **Phase Flux, Dispersed Phase** and choose **Duplicate**.
- 2 In the **Settings** window for **Streamline**, type Phase Flux, Continuous Phase in the **Label** text field.

- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Fluxes > mm.jcr,mm.jcz - Continuous phase flux**.

#### *Mixture Velocity and Phase Flux Streamlines*

In the **Mixture Velocity and Phase Flux Streamlines** toolbar, click  **Annotation**.

#### *Annotation 1*

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type Time = 10 s, Mixture Velocity.
- 3 Locate the **Position** section. In the **r** text field, type -0.035.
- 4 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 5 From the **Orientation** list, choose **Vertical**.
- 6 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

#### *Annotation 2*

- 1 Right-click **Results > Mixture Velocity and Phase Flux Streamlines > Annotation 1** and choose **Duplicate**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Time = 10 s, Dispersed Phase Flux.
- 4 Locate the **Plot Array** section. In the **Index** text field, type 1.

#### *Annotation 3*

- 1 Right-click **Annotation 2** and choose **Duplicate**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Time = 10 s, Continuous Phase Flux.
- 4 Locate the **Plot Array** section. In the **Index** text field, type 2.

#### *Annotation 1, Annotation 2, Annotation 3, Mixture Velocity, Phase Flux, Continuous Phase, Phase Flux, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Mixture Velocity and Phase Flux Streamlines**, Ctrl-click to select **Mixture Velocity, Phase Flux, Dispersed Phase, Phase Flux, Continuous Phase, Annotation 1, Annotation 2, and Annotation 3**.
- 2 Right-click and choose **Duplicate**.

#### *Mixture Velocity 1*

- 1 In the **Settings** window for **Surface**, locate the **Data** section.
- 2 From the **Time (s)** list, choose **210**.

- 3 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Mixture Velocity**.

#### *Phase Flux, Dispersed Phase 1*

- 1 In the **Model Builder** window, click **Phase Flux, Dispersed Phase 1**.
- 2 In the **Settings** window for **Streamline**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **210**.

#### *Phase Flux, Continuous Phase 1*

- 1 In the **Model Builder** window, click **Phase Flux, Continuous Phase 1**.
- 2 In the **Settings** window for **Streamline**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **210**.




#### *Annotation 4*

- 1 In the **Model Builder** window, click **Annotation 4**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Time = 210 s, Mixture Velocity.
- 4 Locate the **Plot Array** section. In the **Index** text field, type 3.

#### *Annotation 5*


- 1 In the **Model Builder** window, click **Annotation 5**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Time = 210 s, Dispersed Phase Flux.
- 4 Locate the **Plot Array** section. In the **Index** text field, type 4.

#### *Annotation 6*

- 1 In the **Model Builder** window, click **Annotation 6**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Time = 210 s, Continuous Phase Flux.
- 4 Locate the **Plot Array** section. In the **Index** text field, type 5.
- 5 In the **Mixture Velocity and Phase Flux Streamlines** toolbar, click  **Plot**.
- 6 Click the  **Show Grid** button in the **Graphics** toolbar.
- 7 Click the  **Zoom Extents** button in the **Graphics** toolbar.


Next, create a plot to show the phase velocities and dispersed phase volume fraction in 3D.

#### *Phase Velocities and Volume Fraction (3D)*


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

- 2 In the **Settings** window for **3D Plot Group**, type **Phase Velocities and Volume Fraction (3D)** in the **Label** text field.
- 3 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.
- 5 Locate the **Color Legend** section. Select the **Show units** checkbox.
- 6 Click to expand the **Plot Array** section. From the **Array type** list, choose **Linear**.
- 7 From the **Padding** list, choose **Absolute**.
- 8 In the **Padding length** text field, type 0.2.

#### *Stages*

- 1 In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **Surface**.
- 2 In the **Settings** window for **Surface**, type **Stages** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Revolution 2D 2**.
- 4 Locate the **Expression** section. In the **Expression** text field, type 1.
- 5 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

#### *Material Appearance 1*

- 1 In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **Material Appearance**.
- 2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
- 3 From the **Appearance** list, choose **Custom**.
- 4 From the **Material type** list, choose **Steel (anodized)**.

#### *Column*

- 1 In the **Model Builder** window, right-click **Stages** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, type **Column** in the **Label** text field.
- 3 Locate the **Data** section. From the **Dataset** list, choose **Revolution 2D 3**.


#### *Phase Velocities and Volume Fraction (3D)*

In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **Surface**.

#### *Velocity, Dispersed Phase*

- 1 In the **Settings** window for **Surface**, type **Velocity, Dispersed Phase** in the **Label** text field.
- 2 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Velocity and pressure > mm.Ud - Velocity field, dispersed phase - m/s**.
- 3 Locate the **Plot Array** section. Select the **Manual indexing** checkbox.


### *Phase Velocities and Volume Fraction (3D)*

In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **More Plots** and choose **Streamline Surface**.

#### *Velocity Field, Dispersed Phase*

- 1 In the **Settings** window for **Streamline Surface**, type Velocity Field, Dispersed Phase in the **Label** text field.
- 2 Locate the **Data** section. From the **Dataset** list, choose **Cut Plane I**.
- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component I (comp1) > Mixture Model, k- $\omega$  > Velocity and pressure > mm.udr,...,mm.udz - Velocity field, dispersed phase**.
- 4 Locate the **Streamline Positioning** section. From the **Positioning** list, choose **Uniform density**.
- 5 In the **Density level** text field, type 8.5.
- 6 Locate the **Coloring and Style** section. Find the **Line style** subsection. From the **Type** list, choose **Tube**.
- 7 Select the **Radius scale factor** checkbox. In the associated text field, type 0.0015.
- 8 Find the **Point style** subsection. From the **Type** list, choose **Arrow**.
- 9 Select the **Scale factor** checkbox. In the associated text field, type 0.2.
- 10 From the **Color** list, choose **Custom**.
- 11 On Windows, click the colored bar underneath, or — if you are running the cross-platform desktop — the **Color** button.
- 12 Click **Define custom colors**.
- 13 Set the RGB values to 255, 160, and 122, respectively.
- 14 Click **Add to custom colors**.
- 15 Click **Show color palette only** or **OK** on the cross-platform desktop.
- 16 Click to expand the **Plot Array** section. Select the **Manual indexing** checkbox.

### *Phase Velocities and Volume Fraction (3D)*

In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **Annotation**.

#### *Annotation 1*

- 1 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 2 In the **Text** text field, type Dispersed Phase Velocity.
- 3 Locate the **Position** section. In the **x** text field, type  $1.5 \cdot R_c$ .
- 4 In the **z** text field, type  $H_c/2$ .

- 5 Locate the **Coloring and Style** section. Clear the **Show point** checkbox.
- 6 From the **Anchor point** list, choose **Center**.
- 7 From the **Orientation** list, choose **Vertical**.

*Annotation 1, Column, Stages, Velocity Field, Dispersed Phase, Velocity, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Phase Velocities and Volume Fraction (3D)**, Ctrl-click to select **Stages, Column, Velocity, Dispersed Phase, Velocity Field, Dispersed Phase**, and **Annotation 1**.
- 2 Right-click and choose **Duplicate**.

*Stages 1*

- 1 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 2 In the **Index** text field, type 1.

*Column 1*

- 1 In the **Model Builder** window, click **Column 1**.
- 2 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 3 In the **Index** text field, type 1.

*Velocity, Continuous Phase*

- 1 In the **Model Builder** window, under **Results > Phase Velocities and Volume Fraction (3D)** click **Velocity, Dispersed Phase 1**.
- 2 In the **Settings** window for **Surface**, type Velocity, Continuous Phase in the **Label** text field.
- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Velocity and pressure > mm.Uc - Velocity field, continuous phase - m/s**.
- 4 Click to expand the **Inherit Style** section. From the **Plot** list, choose **Velocity, Dispersed Phase**.
- 5 Locate the **Plot Array** section. In the **Index** text field, type 1.

*Velocity Field, Continuous Phase*

- 1 In the **Model Builder** window, under **Results > Phase Velocities and Volume Fraction (3D)** click **Velocity Field, Dispersed Phase 1**.
- 2 In the **Settings** window for **Streamline Surface**, type Velocity Field, Continuous Phase in the **Label** text field.

- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > Velocity and pressure > mm.ucr,...,mm.ucz - Velocity field, continuous phase.**
- 4 Locate the **Plot Array** section. In the **Index** text field, type 1.

#### *Annotation 2*

- 1 In the **Model Builder** window, click **Annotation 2**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Continuous Phase Velocity.

#### *Annotation 1, Column, Stages, Velocity, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Phase Velocities and Volume Fraction (3D)**, Ctrl-click to select **Stages, Column, Velocity, Dispersed Phase, and Annotation 1**.
- 2 Right-click and choose **Duplicate**.

#### *Stages 2*

- 1 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 2 In the **Index** text field, type 2.

#### *Column 2*



- 1 In the **Model Builder** window, click **Column 2**.
- 2 In the **Settings** window for **Surface**, locate the **Plot Array** section.
- 3 In the **Index** text field, type 2.

#### *Volume Fraction, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Phase Velocities and Volume Fraction (3D)** click **Velocity, Dispersed Phase 1**.
- 2 In the **Settings** window for **Surface**, type Volume Fraction, Dispersed Phase in the **Label** text field.
- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Mixture Model, k- $\omega$  > mm.phidReg - Volume fraction, dispersed phase - 1**.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **AuroraBorealis**.
- 5 Locate the **Plot Array** section. In the **Index** text field, type 2.

#### *Annotation 3*

- 1 In the **Model Builder** window, click **Annotation 3**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.

- 3 In the **Text** text field, type Dispersed Phase Volume Fraction.
- 4 In the **Phase Velocities and Volume Fraction (3D)** toolbar, click  **Plot**.
- 5 Click the  **Zoom Extents** button in the **Graphics** toolbar.

Create a second 3D plot group to show the phase concentrations and the solute extraction rate.

#### *Phase Concentrations and Solute Extraction Rate (3D)*

- 1 In the **Model Builder** window, right-click **Phase Velocities and Volume Fraction (3D)** and choose **Duplicate**.
- 2 In the **Settings** window for **3D Plot Group**, type Phase Concentrations and Solute Extraction Rate (3D) in the **Label** text field.
- 3 In the **Model Builder** window, expand the **Phase Concentrations and Solute Extraction Rate (3D)** node.

#### *Velocity Field, Continuous Phase, Velocity Field, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Phase Concentrations and Solute Extraction Rate (3D)**, Ctrl-click to select **Velocity Field, Dispersed Phase** and **Velocity Field, Continuous Phase**.
- 2 Right-click and choose **Delete**.

#### *Concentration, Dispersed Phase*

- 1 In the **Model Builder** window, under **Results > Phase Concentrations and Solute Extraction Rate (3D)** click **Velocity, Dispersed Phase**.
- 2 In the **Settings** window for **Surface**, type Concentration, Dispersed Phase in the **Label** text field.
- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Dispersed Phase Transport of Diluted Species 2 > Species cd > tds2.phs\_cd - Phase specific concentration - mol/m<sup>3</sup>**.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **Prism**.

#### *Annotation 1*

- 1 In the **Model Builder** window, click **Annotation 1**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Concentration, Dispersed Phase.

#### *Concentration, Continuous Phase*

- 1 In the **Model Builder** window, under **Results > Phase Concentrations and Solute Extraction Rate (3D)** click **Velocity, Continuous Phase**.

- 2 In the **Settings** window for **Surface**, type Concentration, Continuous Phase in the **Label** text field.
- 3 Click **Replace Expression** in the upper-right corner of the **Expression** section. From the menu, choose **Component 1 (comp1) > Continuous Phase Transport of Diluted Species > Species cc > tds.phs\_cc - Phase specific concentration - mol/m<sup>3</sup>**.


#### *Annotation 2*

- 1 In the **Model Builder** window, click **Annotation 2**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Concentration, Continuous Phase.

#### *Solute Extraction Rate*


- 1 In the **Model Builder** window, under **Results > Phase Concentrations and Solute Extraction Rate (3D)** click **Volume Fraction, Dispersed Phase**.
- 2 In the **Settings** window for **Surface**, type Solute Extraction Rate in the **Label** text field.
- 3 Locate the **Expression** section. In the **Expression** text field, type `dds1.Re_cc`.
- 4 Locate the **Coloring and Style** section. From the **Color table** list, choose **JupiterAuroraBorealis**.

#### *Annotation 3*

- 1 In the **Model Builder** window, click **Annotation 3**.
- 2 In the **Settings** window for **Annotation**, locate the **Annotation** section.
- 3 In the **Text** text field, type Solute Extraction Rate.
- 4 In the **Phase Concentrations and Solute Extraction Rate (3D)** toolbar, click  **Plot**.

Create a plot to show the column geometry in 3D.

#### *Geometry*


- 1 In the **Results** toolbar, click  **3D Plot Group**.
- 2 In the **Settings** window for **3D Plot Group**, type Geometry in the **Label** text field.
- 3 Locate the **Title** section. From the **Title type** list, choose **None**.
- 4 Locate the **Plot Settings** section. Clear the **Plot dataset edges** checkbox.

#### *Stages*


- 1 In the **Geometry** toolbar, click  **Surface**.
- 2 In the **Settings** window for **Surface**, locate the **Expression** section.

- 3 In the **Expression** text field, type 1.
- 4 Locate the **Data** section. From the **Dataset** list, choose **Revolution 2D 2**.
- 5 In the **Label** text field, type Stages.

#### *Material Appearance 1*


- 1 In the **Geometry** toolbar, click  **Material Appearance**.
- 2 In the **Settings** window for **Material Appearance**, locate the **Appearance** section.
- 3 From the **Appearance** list, choose **Custom**.
- 4 From the **Material type** list, choose **Steel (anodized)**.

#### *Column*


- 1 In the **Model Builder** window, right-click **Stages** and choose **Duplicate**.
- 2 In the **Settings** window for **Surface**, locate the **Data** section.
- 3 From the **Dataset** list, choose **Revolution 2D 3**.
- 4 In the **Label** text field, type Column.
- 5 In the **Geometry** toolbar, click  **Plot**.

Next, create a set of 1D plots to show the total phase concentrations and boundary fluxes.

#### *Evaluation Group 1*


In the **Results** toolbar, click  **Evaluation Group**.

#### *Surface Integration 1*

- 1 In the **Evaluation Group 1** toolbar, click  **Integration** and choose **Surface Integration**.
- 2 In the **Settings** window for **Surface Integration**, locate the **Selection** section.
- 3 From the **Selection** list, choose **Column interior**.
- 4 Locate the **Expressions** section. In the table, enter the following settings:

<b>Expression</b>	<b>Unit</b>	<b>Description</b>
cc	mol	Amount, Continuous Phase
cd	mol	Amount, Dispersed Phase

Evaluate the expressions and plot them in a table graph.

- 5 In the **Evaluation Group 1** toolbar, click  **Evaluate**.

#### *1D Plot Group 5*

In the **Evaluation Group 1** toolbar, click  **Table Graph**.

### Table Graph 1

- 1 In the **Settings** window for **Table Graph**, click to expand the **Coloring and Style** section.
- 2 From the **Width** list, choose **2**.
- 3 Click to expand the **Legends** section. Select the **Show legends** checkbox.
- 4 From the **Legends** list, choose **Manual**.
- 5 In the table, enter the following settings:

---

<b>Legends</b>
Continuous Phase
Dispersed Phase

---


### ID Plot Group 5

- 1 In the **Model Builder** window, click **ID Plot Group 5**.
- 2 In the **Settings** window for **ID Plot Group**, click to expand the **Plot Settings** section.
- 3 Select the **y-axis label** checkbox. In the associated text field, type Amount (mol).
- 4 Locate the **Legend** section. From the **Position** list, choose **Upper left**.

### Evaluation Group 2

In the **Results** toolbar, click  **Evaluation Group**.

### Line Integration 1

- 1 In the **Evaluation Group 2** toolbar, click  **Integration** and choose **Line Integration**.
- 2 Select Boundary 2 only.
- 3 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 4 In the table, enter the following settings:

---

<b>Expression</b>	<b>Unit</b>	<b>Description</b>
mm.jdz*mm.nz	m <sup>3</sup> /s	Bottom inlet

---

### Evaluation Group 2

In the **Evaluation Group 2** toolbar, click  **Integration** and choose **Line Integration**.

### Line Integration 2

- 1 Select Boundary 36 only.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.

3 In the table, enter the following settings:

Expression	Unit	Description
mm.jdz*mm.nz	m <sup>3</sup> /s	Bottom outlet

#### Evaluation Group 2

In the **Evaluation Group 2** toolbar, click  **Integration** and choose **Line Integration**.

#### Line Integration 3

- 1 Select Boundary 19 only.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jdz*mm.nz	m <sup>3</sup> /s	Top inlet


#### Evaluation Group 2

In the **Evaluation Group 2** toolbar, click  **Integration** and choose **Line Integration**.

#### Line Integration 4

- 1 Select Boundary 42 only.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jdz*mm.nz	m <sup>3</sup> /s	Top outlet

- 4 In the **Evaluation Group 2** toolbar, click  **Evaluate**.

#### ID Plot Group 6

In the **Evaluation Group 2** toolbar, click  **Table Graph**.

#### Table Graph 1

- 1 In the **Settings** window for **Table Graph**, locate the **Legends** section.
- 2 Select the **Show legends** checkbox.

#### ID Plot Group 6

- 1 In the **Model Builder** window, click **ID Plot Group 6**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Upper left**.

### Evaluation Group 3

In the **Model Builder** window, under **Results** right-click **Evaluation Group 2** and choose **Duplicate**.

#### Line Integration 1

- 1 In the **Model Builder** window, expand the **Evaluation Group 3** node, then click **Line Integration 1**.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jcz*mm.nz	m <sup>3</sup> /s	Bottom inlet

#### Line Integration 2

- 1 In the **Model Builder** window, click **Line Integration 2**.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jcz*mm.nz	m <sup>3</sup> /s	Bottom outlet

#### Line Integration 3

- 1 In the **Model Builder** window, click **Line Integration 3**.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jcz*mm.nz	m <sup>3</sup> /s	Top inlet

#### Line Integration 4

- 1 In the **Model Builder** window, click **Line Integration 4**.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
mm.jcz*mm.nz	m <sup>3</sup> /s	Top outlet

- 4 In the **Evaluation Group 3** toolbar, click  **Evaluate**.

### *ID Plot Group 7*

In the **Evaluation Group 3** toolbar, click  **Table Graph**.


### *Table Graph 1*

- 1 In the **Settings** window for **Table Graph**, locate the **Legends** section.
- 2 Select the **Show legends** checkbox.


### *ID Plot Group 7*

- 1 In the **Model Builder** window, click **ID Plot Group 7**.
- 2 In the **Settings** window for **ID Plot Group**, locate the **Legend** section.
- 3 From the **Position** list, choose **Upper left**.

### *Evaluation Group 4*

In the **Results** toolbar, click  **Evaluation Group**.

### *Line Integration 1*

- 1 In the **Evaluation Group 4** toolbar, click  **Integration** and choose **Line Integration**.
- 2 Select Boundary 2 only.
- 3 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 4 In the table, enter the following settings:

Expression	Unit	Description
-tds2.ntflux_cd	mol/s	Dispersed phase, species inflow

- 5 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.
- 6 Select the **Cumulative** checkbox.

### *Evaluation Group 4*


In the **Evaluation Group 4** toolbar, click  **Integration** and choose **Line Integration**.

### *Line Integration 2*

- 1 Select Boundaries 2, 36, and 42 only.
- 2 In the **Settings** window for **Line Integration**, locate the **Expressions** section.
- 3 In the table, enter the following settings:

Expression	Unit	Description
tds.ntflux_cc	mol/s	Continuous phase, species outflow

- 4 Locate the **Data Series Operation** section. From the **Transformation** list, choose **Integral**.
- 5 Select the **Cumulative** checkbox.

6 In the **Evaluation Group 4** toolbar, click  **Evaluate**.

#### *ID Plot Group 8*

In the **Evaluation Group 4** toolbar, click  **Table Graph**.

#### *Table Graph 1*

1 In the **Settings** window for **Table Graph**, click to expand the **Coloring and Style** section.

2 From the **Width** list, choose **2**.

3 Locate the **Legends** section. Select the **Show legends** checkbox.

4 From the **Legends** list, choose **Manual**.

5 In the table, enter the following settings:

<b>Legends</b>
Dispersed phase, species inflow
Continuous phase, species outflow


#### *ID Plot Group 8*

1 In the **Model Builder** window, click **ID Plot Group 8**.

2 In the **Settings** window for **ID Plot Group**, locate the **Plot Settings** section.

3 Select the **y-axis label** checkbox. In the associated text field, type Amount (mol).

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

5 In the **ID Plot Group 8** toolbar, click  **Plot**.

#### *ID Plot Group 5, Evaluation Group 1*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **ID Plot Group 5** and **Evaluation Group 1**.

2 Right-click and choose **Group**.

#### *Phase Concentrations*

In the **Settings** window for **Group**, type Phase Concentrations in the **Label** text field.

#### *ID Plot Group 6, Evaluation Group 2*

1 In the **Model Builder** window, under **Results**, Ctrl-click to select **ID Plot Group 6** and **Evaluation Group 2**.

2 Right-click and choose **Group**.

#### *Boundary Fluxes, Dispersed Phase*

In the **Settings** window for **Group**, type Boundary Fluxes, Dispersed Phase in the **Label** text field.

*ID Plot Group 7, Evaluation Group 3*

**1** In the **Model Builder** window, under **Results**, Ctrl-click to select **ID Plot Group 7** and **Evaluation Group 3**.

**2** Right-click and choose **Group**.

*Boundary Fluxes, Continuous Phase*

In the **Settings** window for **Group**, type Boundary Fluxes, Continuous Phase in the **Label** text field.

*ID Plot Group 8, Evaluation Group 4*

**1** In the **Model Builder** window, under **Results**, Ctrl-click to select **ID Plot Group 8** and **Evaluation Group 4**.

**2** Right-click and choose **Group**.

*Species Boundary Fluxes*

In the **Settings** window for **Group**, type Species Boundary Fluxes in the **Label** text field.