Created in COMSOL Multiphysics 5.6

Separation Through Electrocoalescence

Introduction

A mixture of immiscible liquids is known as an emulsion. Many chemical processes result in emulsions consisting of the desired product and a solvent. Droplets of most emulsions will coalesce given enough time, but it is often desirable to speed up the separation process.

If the liquids have different electric permittivities, an electric field can be applied across the emulsion to stimulate coalescence. This method, known as electrocoalescence, has important applications, for instance, in the separation of oil from water.

To model electrocoalescence, you need to solve the Navier-Stokes equations, describing the fluid motion, as well as track the interfaces between the immiscible fluids. In order to include the electric forces acting on the fluids, you also have to solve for the local electric field. This complex multiphysics process can readily be set up and solved with COMSOL Multiphysics.

Model Definition

GEOMETRY

Two droplets of water with radii of 1.6 and 1.2 mm, respectively, are transported in an oil phase flowing between two parallel plates. The average velocity of the multiphase flow is 5 cm/s. An electric potential of 5 kV is applied over the plates.

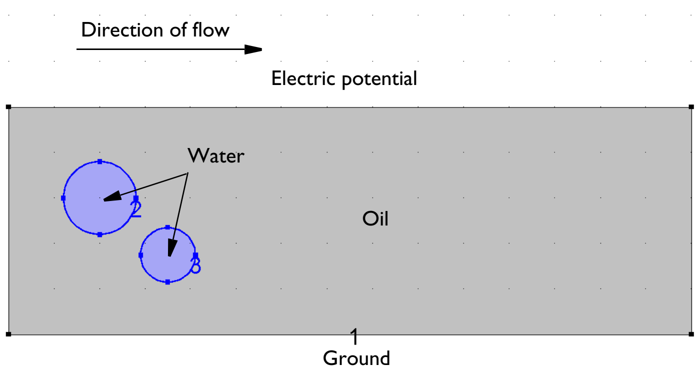

Figure 1: Two water droplets are transported in an oil phase flowing between two plates.

THE TWO PHASE FLOW PHASE FIELD INTERFACE

The Laminar Two-Phase Flow, Phase Field interface sets up the equations for the fluid motion according to the Navier-Stokes equations:

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

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

where $\mathbf{u}$ denotes velocity (SI unit: m/s), ρ the density (SI unit: kg/m^3), μ dynamic viscosity (SI unit: Pas), p pressure (SI unit: Pa), $\mathbf{g}$ gravity (SI unit: m/s^2). $\mathbf{F}_{st}$ is the surface tension force (SI unit: N/m^3), and $\mathbf{F}$ is any additional volume force (SI unit: N/m^3).

To track the fluid interface, the Laminar Two-Phase Flow, Phase Field interface uses a phase field method:

$$\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi = \nabla\cdot\frac{3\chi\sigma\varepsilon}{2\sqrt{2}}\nabla\psi$$

$$\psi = -\nabla\cdot\varepsilon^2\nabla\phi + (\phi^2 - 1)\phi$$

The phase field variable ϕ is −1 in water and 1 in oil. The density and viscosity, which is different for oil and water, is automatically calculated from the phase field variable ϕ, as well as the surface tension force. σ is the surface tension coefficient (SI unit: N/m), ε is a numerical parameter (m) that determines the thickness of the fluid interface, that is, the region where the phase field variable varies smoothly from −1 to 1. χ controls the mobility of the interface.

THE ELECTROSTATICS INTERFACE

The Electrostatics interface sets up the following equations for the electric potential V:

$$-\nabla\cdot(\varepsilon_0\varepsilon_r\nabla V) = 0$$

Here, ε_0 is the permittivity of vacuum, and ε_r is the relative permittivity.

THE COUPLING OF THE TWO PHYSICS

The software automatically sets up the equations described in the two previous sections. You only have to specify how they are coupled. For the Two Phase Flow interface, you need to specify the electric force. The electric force is given by the divergence of the Maxwell stress tensor:

$$\mathbf{F} = \nabla\cdot\mathbf{T} \tag{1}$$

The Maxwell stress tensor is given by:

$$\mathbf{T} = \mathbf{E}\mathbf{D}^T - \frac{1}{2}(\mathbf{E}\cdot\mathbf{D})\mathbf{I}$$

where **E** is the electric field and **D** is the electric displacement field:

$$\mathbf{E} = -\nabla V$$

$$\mathbf{D} = \varepsilon_0 \varepsilon_r \mathbf{E}$$

The present example is in 2D, so the stress tensor is:

$$\mathbf{T} = \begin{bmatrix} T_{xx} & T_{xy} \\ T_{yx} & T_{yy} \end{bmatrix} =$$

$$\begin{bmatrix} \varepsilon_0 \varepsilon_r E_x^2 - \frac{1}{2}\varepsilon_0 \varepsilon_r (E_x^2 + E_y^2) & \varepsilon_0 \varepsilon_r E_x E_y \\ \varepsilon_0 \varepsilon_r E_y E_x & \varepsilon_0 \varepsilon_r E_y^2 - \frac{1}{2}\varepsilon_0 \varepsilon_r (E_x^2 + E_y^2) \end{bmatrix}$$

The components of the electric field are calculated by the Electrostatics interface. Their predefined variable names, along with the variable names of the permeabilities can be used directly to set up expressions calculating the component of the stress tensor.

Variables

Name	Expression	Unit	Description
Tem11	-epsilon0_const*epsilon_r/2*(es.Ex^2+es.Ey^2)+epsilon0_const*epsilon_r*es.Ex^2	Pa	Maxwell stress tensor, 11-...
Tem22	-epsilon0_const*epsilon_r/2*(es.Ex^2+es.Ey^2)+epsilon0_const*epsilon_r*es.Ey^2	Pa	Maxwell stress tensor, 22-...
Tem12	epsilon0_const*epsilon_r*es.Ex*es.Ey	Pa	Maxwell stress tensor, 12-...
Tem21	epsilon0_const*epsilon_r*es.Ex*es.Ey	Pa	Maxwell stress tensor, 21-...
Fx	d(Tem11,x)+d(Tem12,y)	N/m³	Force, x-component
Fy	d(Tem21,x)+d(Tem22,y)	N/m³	Force, y-component
epsilon_r	tpf.Vf1*perm_water+tpf.Vf2*perm_oil		Phase dependent permitti...

Figure 2: Use the Variables feature to define expressions. Predefined variables and operators can be typed in directly.

The components of the volume force are given by Equation 1. Once again, these can also be entered directly as expressions in the graphical user interface. Table 1 shows the syntax for the partial derivatives of the stress tensor that express the volume force in the x and y directions.

TABLE 1: USER DEFINED VARIABLES.

NAME	EXPRESSION
Tem11	-epsilon0_const*epsilon_r/2*(es.Ex^2+es.Ey^2)+ epsilon0_const*epsilon_r*es.Ex^2
Tem22	-epsilon0_const*epsilon_r/2*(es.Ex^2+es.Ey^2)+ epsilon0_const*epsilon_r*es.Ey^2
Tem12	epsilon0_const*epsilon_r*es.Ex*es.Ey
Tem21	epsilon0_const*epsilon_r*es.Ex*es.Ey
Fx	d(Tem11,x)+d(Tem12,y)
Fy	d(Tem21,x)+d(Tem22,y)
epsilon_r	tpf.Vf1*perm_water+tpf.Vf2*perm_oil

Finally, you also need to specify the relative permittivity. The relative permittivity is constant, but different, for each fluid. You define it from the internally defined volume fractions of each fluid, `Vf1` and `Vf2`:

$$\varepsilon_r = \varepsilon_{r1}\mathrm{Vf1} + \varepsilon_{r2}\mathrm{Vf2}$$

Here, ε_{r1} and ε_{r2} denote the relative permittivity of oil and water, respectively.

Results and Discussion

Figure 3 shows snapshots of the velocity and water droplets at a 0.05 s interval. Contour lines of the electric potential show a dynamic behavior, clearly illustrating the two-way coupling in this multiphysics problem. The influence of the electric field cause the water droplets to stretch to the point where they come into contact. At this point, surface tension causes the droplets to coalesce. The surface tension forces counteracts the electric forces stretching the newly formed droplet.

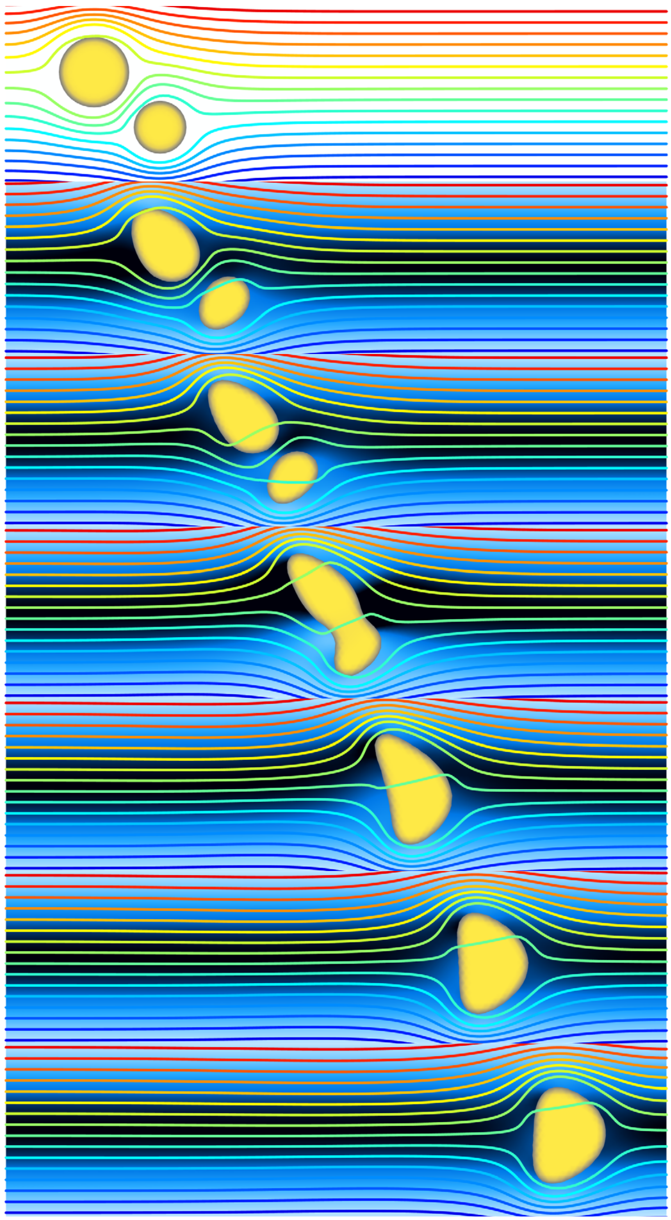

Figure 3: Water droplets, velocity, and the contour lines of the electric potential at 0, 0.05, 0.1, 0.015, 0.2, 0.25, 0.3 seconds.

Application Library path: `CFD_Module/Multiphase_Flow/electrocoalescence`

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 **2D**.

2 In the **Select Physics** tree, select **AC/DC>Electric Fields and Currents>Electrostatics (es)**.

3 Click **Add**.

4 In the **Select Physics** tree, select **Fluid Flow>Multiphase Flow>Two-Phase Flow, Phase Field>Laminar Flow**.

5 Click **Add**.

6 Click **Study**.

7 In the **Select Study** tree, select **Preset Studies for Selected Multiphysics> Time Dependent with Phase Initialization**.

8 Click **Done**.

GEOMETRY 1

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

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

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

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 `30`.

4 In the **Height** text field, type `10`.

Circle 1 (c1)

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

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

3 In the **Radius** text field, type 1.6.

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

5 In the **y** text field, type 6.

Circle 2 (c2)

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

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

3 In the **Radius** text field, type 1.2.

4 Locate the **Position** section. In the **x** text field, type 7.

5 In the **y** text field, type 3.5.

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 In the table, enter the following settings:

Name	Expression	Value	Description
perm_water	80	80	Permittivity, water
perm_oil	2.2	2.2	Permittivity, oil
u_in	50[mm/s]	0.05 m/s	Average inlet velocity
u_max	3/2*u_in	0.075 m/s	Approximated maximum velocity
sigma	0.031[N/m]	0.031 N/m	Surface tension coefficient
V0	5[kV]	5000 V	Applied voltage

DEFINITIONS

Variables 1

1 In the **Home** toolbar, click a= **Variables** and choose **Local Variables**.

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

3 In the table, enter the following settings:

Name	Expression	Unit	Description
`Tem11`	`-epsilon0_const* epsilon_r/2*(es.Ex^2+ es.Ey^2)+epsilon0_const* epsilon_r*es.Ex^2`	Pa	`Maxwell stress tensor, 11-component`
`Tem22`	`-epsilon0_const* epsilon_r/2*(es.Ex^2+ es.Ey^2)+epsilon0_const* epsilon_r*es.Ey^2`	Pa	`Maxwell stress tensor, 22-component`
`Tem12`	`epsilon0_const* epsilon_r*es.Ex*es.Ey`	Pa	`Maxwell stress tensor, 12-component`
`Tem21`	`epsilon0_const* epsilon_r*es.Ex*es.Ey`	Pa	`Maxwell stress tensor, 21-component`
`Fx`	`d(Tem11,x)+d(Tem12,y)`	N/m^3	`Force, x-component`
`Fy`	`d(Tem21,x)+d(Tem22,y)`	N/m^3	`Force, y-component`
`epsilon_r`	`pf.Vf1*perm_water+ pf.Vf2*perm_oil`		`Phase dependent permittivity`

Create a step function which will be used to ramp up the inlet velocity from zero to its full value over the initial 0.01 s.

Step 1 (step1)

1 In the **Home** toolbar, click f(X) **Functions** and choose **Local>Step**.

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

3 In the **Location** text field, type `0.005`.

4 Click to expand the **Smoothing** section. In the **Size of transition zone** text field, type `0.01`.

5 Click **Plot**.

Now, create selections to be used when setting up the boundary conditions.

Outlet

1 In the **Definitions** toolbar, click **Explicit**.

2 Right-click **Explicit 1** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Outlet` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundary 4 only.

Inlet

1 In the **Definitions** toolbar, click **Explicit**.

2 In the **Model Builder** window, right-click **Explicit 2** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Inlet` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundary 1 only.

Oil/Water Interface

1 In the **Definitions** toolbar, click **Explicit**.

2 Right-click **Explicit 3** and choose **Rename**.

3 In the **Rename Explicit** dialog box, type `Oil/Water Interface` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Explicit**, locate the **Input Entities** section.

6 From the **Geometric entity level** list, choose **Boundary**.

7 Select Boundaries 5–12 only.

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 **Liquids and Gases>Liquids>Water**.

4 Click **Add to Component** in the window toolbar.

5 In the **Home** toolbar, click **Add Material** to close the **Add Material** window.

MATERIALS

Oil

1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Materials** and choose **Blank Material**.

2 Right-click **Material 2 (mat2)** and choose **Rename**.

3 In the **Rename Material** dialog box, type `Oil` in the **New label** text field.

4 Click **OK**.

5 In the **Settings** window for **Material**, click to expand the **Material Properties** section.

6 In the **Material properties** tree, select **Basic Properties>Density**.

7 Click **Add to Material**.

8 In the **Material properties** tree, select **Basic Properties>Dynamic Viscosity**.

9 Click **Add to Material**.

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

Property	Variable	Value	Unit	Property group
Density	rho	884[kg/m^3]	kg/m³	Basic
Dynamic viscosity	mu	0.474[Pa*s]	Pa·s	Basic

ELECTROSTATICS (ES)

Charge Conservation 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Electrostatics (es)** click **Charge Conservation 1**.

2 In the **Settings** window for **Charge Conservation**, locate the **Constitutive Relation D-E** section.

3 From the ε_r list, choose **User defined**. In the associated text field, type `epsilon_r`.

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 V text field, type `y*V0/10[mm]`.

Electric Potential 1

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

2 Select Boundary 3 only (top boundary).

3 In the **Settings** window for **Electric Potential**, locate the **Electric Potential** section.

4 In the V_0 text field, type `V0`.

Ground 1

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

2 Select Boundary 2 only (bottom boundary).

MULTIPHYSICS

Two-Phase Flow, Phase Field 1 (tpf1)

1 In the **Model Builder** window, under **Component 1 (comp1)>Multiphysics** click **Two-Phase Flow, Phase Field 1 (tpf1)**.
2 In the **Settings** window for **Two-Phase Flow, Phase Field**, locate the **Fluid 1 Properties** section.
3 From the **Fluid 1** list, choose **Water (mat1)**.
4 Locate the **Fluid 2 Properties** section. From the **Fluid 2** list, choose **Oil (mat2)**.
5 Locate the **Surface Tension** section. From the **Surface tension coefficient** list, choose **User defined**. In the σ text field, type `sigma`.

PHASE FIELD (PF)

Phase Field Model 1

1 In the **Model Builder** window, under **Component 1 (comp1)>Phase Field (pf)** click **Phase Field Model 1**.
2 In the **Settings** window for **Phase Field Model**, locate the **Phase Field Parameters** section.
3 In the ε_{pf} text field, type `0.15[mm]`.
4 From the **Mobility tuning parameter** list, choose **Calculate from velocity**.
5 In the U text field, type `u_max`.

Initial Values, Fluid 2

1 In the **Model Builder** window, click **Initial Values, Fluid 2**.
2 Select Domain 1 only.

LAMINAR FLOW (SPF)

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

Volume Force 1

1 In the **Physics** toolbar, click **Domains** and choose **Volume Force**.
2 In the **Settings** window for **Volume Force**, locate the **Domain Selection** section.
3 From the **Selection** list, choose **All domains**.
4 Locate the **Volume Force** section. Specify the **F** vector as

Fx	x
Fy	y

Inlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.
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 **Fully developed flow**.
5 Locate the **Fully Developed Flow** section. In the U_{av} text field, type `u_in*step1(t*1[1/s])`.

PHASE FIELD (PF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Phase Field (pf)**.
2 In the **Physics** toolbar, click **Boundaries** and choose **Inlet**.

Inlet 1

1 In the **Settings** window for **Inlet**, locate the **Boundary Selection** section.
2 From the **Selection** list, choose **Inlet**.
3 Locate the **Phase Field Condition** section. From the list, choose **Fluid 2 (φ = 1)**.

LAMINAR FLOW (SPF)

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

Outlet 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.
2 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.
3 From the **Selection** list, choose **Outlet**.
4 Locate the **Boundary Condition** section. From the list, choose **Fully developed flow**.

PHASE FIELD (PF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Phase Field (pf)**.
2 In the **Physics** toolbar, click **Boundaries** and choose **Outlet**.

Outlet 1

1 In the **Settings** window for **Outlet**, locate the **Boundary Selection** section.
2 From the **Selection** list, choose **Outlet**.

MESH 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Mesh 1**.
2 In the **Settings** window for **Mesh**, locate the **Physics-Controlled Mesh** section.

3 From the **Element size** list, choose **Fine**.
4 Click **Build All**.

STUDY 1

Step 2: Time Dependent

1 In the **Model Builder** window, under **Study 1** click **Step 2: Time Dependent**.
2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
3 In the **Output times** text field, type `range(0,0.05,0.3)`.

In time-dependent simulations, you should, if possible, scale your variables manually. Do this as follows:

Solution 1 (sol1)

1 In the **Study** toolbar, click **Show Default Solver**.
2 In the **Model Builder** window, expand the **Solution 1 (sol1)** node, then click **Dependent Variables 2**.
3 In the **Settings** window for **Dependent Variables**, locate the **Scaling** section.
4 From the **Method** list, choose **Manual**.
5 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1 (sol1)>Dependent Variables 2** node, then click **Electric potential (comp1.V)**.
6 In the **Settings** window for **Field**, locate the **Scaling** section.
7 From the **Method** list, choose **Manual**.
8 In the **Scale** text field, type `1e3`.
9 In the **Model Builder** window, click **Velocity field (comp1.u)**.
10 In the **Settings** window for **Field**, locate the **Scaling** section.
11 From the **Method** list, choose **Manual**.
12 In the **Scale** text field, type `u_max`.

Next, couple the Electrostatics and Velocity u, Pressure p segregated groups.

13 In the **Model Builder** window, expand the **Study 1>Solver Configurations>Solution 1 (sol1)>Time-Dependent Solver 1>Segregated 1** node, then click **Velocity u, Pressure p**.
14 In the **Settings** window for **Segregated Step**, locate the **General** section.
15 Under **Variables**, click **Add**.
16 In the **Add** dialog box, select **Electric potential (comp1.V)** in the **Variables** list.

17 Click **OK**.

18 In the **Model Builder** window, right-click **Electrostatics** and choose **Disable**.

You are now ready to compute the solution:

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

RESULTS

Velocity (spf)

1. In the **Model Builder** window, under **Results** click **Velocity (spf)**.
2. In the **Settings** window for **2D Plot Group**, locate the **Plot Settings** section.
3. Clear the **Plot dataset edges** check box.

Velocity

1. In the **Model Builder** window, expand the **Velocity (spf)** node, then click **Surface**.
2. In the **Settings** window for **Surface**, type `Velocity` in the **Label** text field.
3. Click to expand the **Range** section. Select the **Manual color range** check box.
4. In the **Maximum** text field, type `u_max`.
5. Locate the **Coloring and Style** section. From the **Color table** list, choose **JupiterAuroraBorealis**.
6. Select the **Reverse color table** check box.

Volume Fraction of Fluid

1. In the **Model Builder** window, right-click **Velocity (spf)** and choose **Surface**.
2. In the **Settings** window for **Surface**, type `Volume Fraction of Fluid` in the **Label** text field.
3. Locate the **Expression** section. In the **Expression** text field, type `tpf1.Vf1`.
4. Locate the **Range** section. Select the **Manual data range** check box.
5. In the **Minimum** text field, type `0.5`.
6. In the **Maximum** text field, type `1`.
7. Locate the **Coloring and Style** section. From the **Color table** list, choose **Cividis**.
8. Clear the **Color legend** check box.

Electric potential

1. Right-click **Velocity (spf)** and choose **Contour**.
2. In the **Settings** window for **Contour**, type `Electric potential` in the **Label** text field.
3. Locate the **Coloring and Style** section. From the **Contour type** list, choose **Tube**.

4 In the **Tube radius expression** text field, type `0.06`.

5 Select the **Radius scale factor** check box.

6 Clear the **Color legend** check box.

7 In the **Velocity (spf)** toolbar, click **Plot**.

Velocity (spf)

1 In the **Model Builder** window, click **Velocity (spf)**.

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

3 From the **Time (s)** list, choose **0**.

4 In the **Velocity (spf)** toolbar, click **Plot**.

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

Similarly, plot the solution for the times 0.05, 0.1, 0.15, 0.2, 0.25, and 0.3 s to reproduce the remaining plots in Figure 3.