

Separation Through Electrocoalescence

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, and 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.

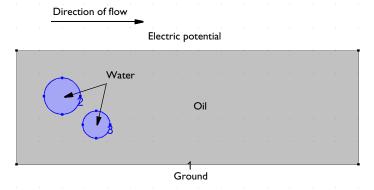


Figure 1: Two water droplets are transported in an oil phase flowing between two plates.

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 **u** denotes velocity (SI unit: m/s), ρ the density (SI unit: kg/m³), μ dynamic viscosity (SI unit: Pas), p pressure (SI unit: Pa), **g** gravity (SI unit: m/s²). \mathbf{F}_{st} is the surface tension force (SI unit: N/m³), and \mathbf{F} is any additional volume force (SI unit: N/m³).

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 \mathbf{E} is the electric field and \mathbf{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:

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

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

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.

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 I: USER DEFINED VARIABLES.

NAME EXPRESSION			
Tem11	-epsilon0_const*es.epsilonr_iso/2*(es.Ex^2+es.Ey^2)+ epsilon0_const*es.epsilonr_iso*es.Ex^2		
Tem22	-epsilonO_const*es.epsilonr_iso/2*(es.Ex^2+es.Ey^2)+ epsilonO_const*es.epsilonr_iso*es.Ey^2		

TABLE I: USER DEFINED VARIABLES.

NAME	EXPRESSION
Tem12	epsilonO_const*es.epsilonr_iso*es.Ex*es.Ey
Tem21	epsilonO_const*es.epsilonr_iso*es.Ex*es.Ey
Fx	d(Tem11,x)+d(Tem12,y)
Fy	d(Tem21,x)+d(Tem22,y)

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

$$\varepsilon_{r} = \varepsilon_{r1}Vf1 + \varepsilon_{r2}Vf2$$

Here, ε_{r1} and ε_{r2} denote the relative permittivity of oil and water, respectively. Instead of using a user-defined variable, this model uses the Multiphase Material to define the effective material properties. This way, the variable es.epsilonr iso in the electrostatics interface is already the correct averaged material property.

Results and Discussion

Figure 3 shows snapshots of the velocity and water droplets at 0.05 s intervals. Contour lines of the electric potential show a dynamic behavior, clearly illustrating the bidirectional coupling in this multiphysics problem. The influence of the electric field causes 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 counteract the electric forces stretching the newly formed droplet.

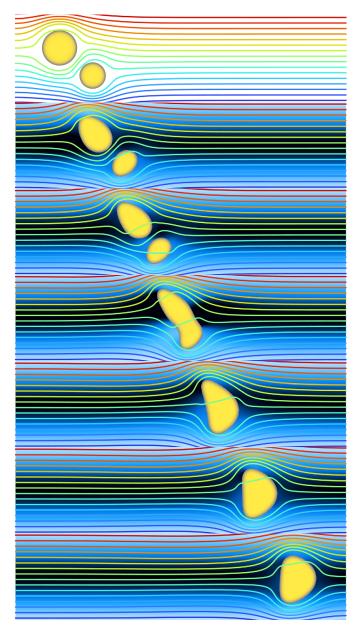


Figure 3: Water droplets, velocity, and the contour lines of the electric potential at 0, 0.05, 0.1, 0.015, 0.2, 0.25, 0.3 seconds.

Application Library path: Microfluidics Module/Two-Phase Flow/ electrocoalescence

Modeling Instructions

From the File menu, choose New.

In the New window, click Model Wizard.

MODEL WIZARD

- I In the Model Wizard window, click **2** 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 M Done.

GEOMETRY I

- I In the Model Builder window, under Component I (compl) click Geometry I.
- 2 In the Settings window for Geometry, locate the Units section.
- 3 From the Length unit list, choose mm.

Rectangle I (rI)

- I 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 I (c1)

- I 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)

- I 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

- I In the Model Builder window, under Global Definitions click Parameters I.
- 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

- I In the Home toolbar, click ∂ = 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	<pre>-epsilon0_const* es.epsilonr_iso/2* (es.Ex^2+es.Ey^2)+ epsilon0_const* es.epsilonr_iso*es.Ex^2</pre>	Pa	Maxwell stress tensor, 11-component
Tem22	<pre>-epsilon0_const* es.epsilonr_iso/2* (es.Ex^2+es.Ey^2)+ epsilon0_const* es.epsilonr_iso*es.Ey^2</pre>	Pa	Maxwell stress tensor, 22-component
Tem12	<pre>epsilon0_const* es.epsilonr_iso*es.Ex* es.Ey</pre>	Pa	Maxwell stress tensor, 12-component
Tem21	<pre>epsilon0_const* es.epsilonr_iso*es.Ex* es.Ey</pre>	Pa	Maxwell stress tensor, 21-component
Fx	d(Tem11,x)+d(Tem12,y)	N/m³	Force, x-component
Fy	d(Tem21,x)+d(Tem22,y)	N/m³	Force, y-component

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 I (step I)

- I 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

- I In the **Definitions** toolbar, click 🔓 **Explicit**.
- 2 In the Settings window for Explicit, type Outlet in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- **4** Select Boundary 4 only.

Inlet

- I In the **Definitions** toolbar, click **\(\bigcap_{\text{a}} \) Explicit**.
- 2 In the Settings window for Explicit, type Inlet in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- 4 Select Boundary 1 only.

Oil/Water Interface

- I In the **Definitions** toolbar, click **\(\bigcap_{\bigcap} \) Explicit**.
- 2 In the Settings window for Explicit, type Oil/Water Interface in the Label text field.
- 3 Locate the Input Entities section. From the Geometric entity level list, choose Boundary.
- **4** Select Boundaries 5–12 only.

ELECTROSTATICS (ES)

Initial Values 1

- I In the Model Builder window, under Component I (compl)>Electrostatics (es) 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 I

- I 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

- I In the Physics toolbar, click Boundaries and choose Ground.
- 2 Select Boundary 2 only (bottom boundary).

MULTIPHYSICS

Two-Phase Flow, Phase Field I (tpfl)

- I In the Model Builder window, under Component I (compl)>Multiphysics click Two-Phase Flow, Phase Field I (tpfI).
- 2 In the Settings window for Two-Phase Flow, Phase Field, locate the Surface Tension section.

- 3 From the Surface tension coefficient list, choose User defined. In the σ text field, type
- 4 Locate the Material Properties section. Click 4 Add Multiphase Material.

MATERIALS

Phase I (mpmat1.phase1)

- I In the Model Builder window, under Component I (compl)>Materials> Multiphase Material I (mpmatl) click Phase I (mpmatl.phasel).
- 2 In the Settings window for Phase, locate the Link Settings section.
- 3 Click 44 Add Material from Library. This button is found when expanding the options next to the Material list.

ADD MATERIAL TO PHASE I (MPMATI.PHASEI)

- I Go to the Add Material to Phase I (mpmat1.phase1) window.
- 2 In the tree, select Liquids and Gases>Liquids>Water.
- 3 Click OK.

GLOBAL DEFINITIONS

Water (mat I)

- I In the Model Builder window, under Global Definitions>Materials click Water (mat1).
- 2 In the Settings window for Material, locate the Material Contents section.
- **3** In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso; epsilonrii = epsilonr_iso, epsilonrij = 0	perm_wa ter	I	Basic

MATERIALS

Phase 2 (mpmat1.phase2)

- I In the Model Builder window, under Component I (compl)>Materials> Multiphase Material I (mpmat I) click Phase 2 (mpmat I.phase 2).
- 2 In the Settings window for Phase, locate the Link Settings section.

3 Click Blank Material. This button is found when expanding the options next to the Material list.

GLOBAL DEFINITIONS

Oil

- I In the Model Builder window, under Global Definitions>Materials click Material 2 (mat2).
- 2 In the Settings window for Material, type 011 in the Label text field.
- **3** Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Relative permittivity	epsilonr_iso; epsilonrii = epsilonr_iso, epsilonrij = 0	perm_oil	I	Basic
Density	rho	884[kg/ m^3]	kg/m³	Basic
Dynamic viscosity	mu	0.474[Pa *s]	Pa·s	Basic

PHASE FIELD IN FLUIDS (PF)

Phase Field Model I

- I In the Model Builder window, under Component I (compl)>Phase Field in Fluids (pf) click Phase Field Model I.
- 2 In the Settings window for Phase Field Model, locate the Phase Field Parameters section.
- **3** In the $\varepsilon_{\rm pf}$ 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

- I 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 I (compl) click Laminar Flow (spf).

Volume Force 1

I 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 \mathbf{F} vector as



Inlet 1

- I 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 $U_{\rm av}$ text field, type u_in*step1(t*1[1/ s]).

PHASE FIELD IN FLUIDS (PF)

- I In the Model Builder window, under Component I (compl) click Phase Field in Fluids (pf).
- 2 In the Physics toolbar, click Boundaries and choose Inlet.
- I 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 ($\varphi = 1$).

LAMINAR FLOW (SPF)

In the Model Builder window, under Component I (compl) click Laminar Flow (spf).

Outlet I

- I 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 IN FLUIDS (PF)

- I In the Model Builder window, under Component I (compl) click Phase Field in Fluids (pf).
- 2 In the Physics toolbar, click Boundaries and choose Outlet.
- I In the Settings window for Outlet, locate the Boundary Selection section.

2 From the **Selection** list, choose **Outlet**.

MESH I

- I In the Model Builder window, under Component I (compl) click Mesh I.
- 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 I

Step 2: Time Dependent

- I In the Model Builder window, under Study I 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 I (soll)

- I In the Study toolbar, click Show Default Solver.
- 2 In the Model Builder window, expand the Solution I (soll) 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 I>Solver Configurations> Solution I (soll)>Dependent Variables 2 node, then click Electric potential (compl.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, under Study I>Solver Configurations>Solution I (soll)> Dependent Variables 2 click Velocity field (compl.u).
- 10 In the Settings window for Field, locate the Scaling section.
- II 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 I (soll)>Time-Dependent Solver I>Segregated I 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 (compl.V) in the Variables list.
- 17 Click OK.
- 18 In the Model Builder window, under Study I>Solver Configurations>Solution I (soll)> Time-Dependent Solver I>Segregated I right-click Electrostatics and choose Disable.

You are now ready to compute the solution:

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

RESULTS

Velocity (sbf)

- I 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

- I 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. Click Change Color Table.
- **6** In the **Color Table** dialog box, select **Aurora>JupiterAuroraBorealis** in the tree.
- 7 Click OK.
- 8 In the Settings window for Surface, locate the Coloring and Style section.
- **9** From the Color table transformation list, choose Reverse.

Volume Fraction of Fluid

- I 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. Click Change Color Table.
- 8 In the Color Table dialog box, select Linear>Cividis in the tree.
- 9 Click OK.
- 10 In the Settings window for Surface, locate the Coloring and Style section.
- II Clear the Color legend check box.

Electric potential

- I 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)

- I 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.