

# Droplet Breakup in a T-Junction

# Introduction

Emulsions consist of small liquid droplets immersed in another liquid, typically oil in water or water in oil. Emulsions find wide application in the production of food, cosmetics, and pharmaceutical products. The properties and quality of an emulsion typically depend on the size and the distribution off the droplets. This example studies in detail how to create uniform droplets in a microchannel T-junction.

Setting up the model you can make use of the multiphysics coupling feature Laminar Two-Phase Flow, Level Set interface. The model uses the multiphysics coupling wetted wall boundary condition at the solid walls, with a contact angle of 135°. From the results, you can determine the size of the created droplets and the rate with which they are produced.

# Model Definition

Figure 1 shows the geometry of the T-shaped microchannel with a rectangular cross section. For the separated fluid elements to correspond to droplets, the geometry is modeled in 3D. Due to symmetry, it is sufficient to model only half of the junction geometry. The modeling domain is shown in Figure 1. The fluid to be dispersed into small droplets, Fluid 2, enters through the vertical channel. The other fluid, Fluid 1, flows from the right to left through the horizontal channel.



Figure 1: The modeling domain of the T-junction.

The problem described is straightforward to set up with the Laminar Two-Phase Flow, Level Set multiphysics coupling feature. The coupling couples the Laminar Flow and Level Set physics interfaces.

The Laminar Flow interface sets up a momentum transport equation and a continuity equation. The Level Set interface sets up a level set equation for the level set variable. The fluid interface is defined by the 0.5 contour of the level set function.

The Laminar Flow and Level Set interfaces use the following equations:

$$\rho \frac{\partial \mathbf{u}}{\partial t} + \rho(\mathbf{u} \cdot \nabla)\mathbf{u} = \nabla \cdot [-p\mathbf{I} + \mu(\nabla \mathbf{u} + (\nabla \mathbf{u})^T)] + \mathbf{F}_{st}$$
$$\nabla \cdot \mathbf{u} = 0$$
$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = \gamma \nabla \cdot \left(-\phi(1-\phi)\frac{\nabla \phi}{|\nabla \phi|} + \varepsilon \nabla \phi\right)$$

In the equations above,  $\rho$  denotes density (kg/m<sup>3</sup>), **u** velocity (m/s), *t* time (s),  $\mu$  dynamic viscosity (Pa·s), *p* pressure (Pa), and **F**<sub>st</sub> the surface tension force (N/m<sup>3</sup>). Furthermore,  $\phi$  is the level set function, and  $\gamma$  and  $\varepsilon$  are numerical stabilization parameters.

The multiphysics coupling feature defines the density and viscosity according to

$$\rho = \rho_1 + (\rho_2 - \rho_1)\phi$$
$$\mu = \mu_1 + (\mu_2 - \mu_1)\phi$$

where  $\rho_1$ ,  $\rho_2$ ,  $\mu_1$ , and  $\mu_2$  are the densities and viscosities of Fluid 1 and Fluid 2. Other definitions of the viscosity and pressure are also available.

# PHYSICAL PARAMETERS

The two liquids have the following physical properties:

QUANTITY	VALUE, FLUID I	VALUE, FLUID 2
Density (kg/m <sup>3</sup> )	1000	1000
Dynamic viscosity (Pa·s)	0.00195	0.00671

The surface tension coefficient is  $5 \cdot 10^{-3}$  N/m.

# **BOUNDARY CONDITIONS**

At both inlets, Fully developed flow conditions with prescribed volume flows are used. At the outflow boundary, the Pressure condition is set. The Wetted wall multiphysics

boundary condition applies to all solid boundaries with the contact angle specified as  $135^{\circ}$  and a slip length equal 6.5e-5 m. The contact angle is the angle between the fluid interface and the solid wall at points where the fluid interface attaches to the wall. The slip length is the distance to the position outside the wall where the extrapolated tangential velocity component is zero (see Figure 2).



Figure 2: The contact angle,  $\theta$ , and the slip length,  $\beta$ .

# Results and Discussion

Figure 3 shows the fluid interface (the level set function  $\phi = 0.5$ ) and velocity streamlines at various times. The first droplet is formed after approximately 0.03 s.



Figure 3: Velocity streamlines and the phase boundary at t = 0.02 s, 0.04 s, 0.06 s, and 0.08 s.

You can calculate the effective diameter,  $d_{\text{eff}}$ — that is, the diameter of a spherical droplet with the same volume as the formed droplet — using the following expression:

$$d_{\rm eff} = 2 \cdot \sqrt[3]{\frac{3}{4\pi} \int_{\Omega} (\phi > 0.5) d\Omega}$$
(1)

Here,  $\Omega$  represents the leftmost part of the horizontal channel, where x < -0.2 mm. In this case, the results show that  $d_{\text{eff}}$  is about 0.12 mm. The results are in fair agreement with those presented in Ref. 1.

# Notes About the COMSOL Implementation

In time dependent problems it is important to respect the CFL condition (Courant-Friedrichs-Lewy condition) to ensure accuracy and stability, namely

$$\Delta t = \frac{Ch}{u}$$

where *C* is the Courant number. Since we are using an implicit method, we can work with a Courant number around 1 and use a constant time step of  $6.5 \cdot 10^{-4}$  s.

# Reference

1. S. van der Graaf, T. Nisisako, C.G.P.H. Schroën, R.G.M. van der Sman, and R.M. Boom, "Lattice Boltzmann Simulations of Droplet Formation in a T-Shaped Microchannel," *Langmuir*, vol. 22, pp. 4144–4152, 2006.

**Application Library path:** Microfluidics\_Module/Two-Phase\_Flow/ droplet\_breakup

# Modeling Instructions

From the File menu, choose New.

## NEW

In the New window, click 🙆 Model Wizard.

#### MODEL WIZARD

- I In the Model Wizard window, click 间 3D.
- 2 In the Select Physics tree, select Fluid Flow>Multiphase Flow>Two-Phase Flow, Level Set> Laminar Flow.
- 3 Click Add.
- 4 Click 🔿 Study.
- 5 In the Select Study tree, select Preset Studies for Selected Multiphysics> Time Dependent with Phase Initialization.
- 6 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.

Work Plane I (wp1)

I In the Geometry toolbar, click 📥 Work Plane.

- 2 In the Settings window for Work Plane, locate the Plane Definition section.
- 3 From the Plane list, choose xz-plane.
- 4 Click 📥 Show Work Plane.

# Work Plane I (wpl)>Rectangle I (rl)

- I In the Work Plane toolbar, click 📃 Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Width** text field, type **0.1**.
- 4 In the **Height** text field, type 0.4.
- 5 Locate the **Position** section. In the **yw** text field, type 0.1.

Work Plane 1 (wp1)>Rectangle 2 (r2)

- I In the Work Plane toolbar, click Rectangle.
- 2 In the Settings window for Rectangle, locate the Size and Shape section.
- **3** In the **Height** text field, type **0.1**.
- 4 Locate the Position section. In the xw text field, type -0.7.

Work Plane I (wpI)>Plane Geometry

- I In the Work Plane toolbar, click 📗 Build All.
- 2 Click the 🕂 Zoom Extents button in the Graphics toolbar.

Work Plane I (wpl)>Polygon I (poll)

- I In the Work Plane toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Object Type section.
- 3 From the Type list, choose Open curve.
- 4 Locate the **Coordinates** section. In the table, enter the following settings:

xw (mm)	yw (mm)
0	0.2
0.1	0.2

# 5 Click 틤 Build Selected.

Work Plane I (wpl)>Polygon 2 (pol2)

- I In the Work Plane toolbar, click / Polygon.
- 2 In the Settings window for Polygon, locate the Coordinates section.

**3** In the table, enter the following settings:

xw (mm)	yw (mm)
0.1	0
0.1	0.1

4 Click 틤 Build Selected.

Extrude I (extI)

- In the Model Builder window, under Component I (compl)>Geometry I right-click
  Work Plane I (wpl) and choose Extrude.
- 2 In the Settings window for Extrude, locate the Distances section.
- **3** In the table, enter the following settings:

#### Distances (mm)

0.05

- 4 Click 틤 Build Selected.
- **5** Click the + **Zoom Extents** button in the **Graphics** toolbar.

Form Union (fin)

In the Model Builder window, right-click Form Union (fin) and choose Build Selected.
 The geometry should look like in Figure 1.

# MATERIALS

- Fluid I
- I In the Model Builder window, under Component I (comp1) right-click Materials and choose Blank Material.
- 2 Right-click Material I (matl) and choose Rename.
- 3 In the Rename Material dialog box, type Fluid 1 in the New label text field.
- 4 Click OK.
- 5 In the Settings window for Material, locate the Material Contents section.
- 6 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	1e3[kg/m^3]	kg/m³	Basic
Dynamic viscosity	mu	1.95e-3[Pa*s]	Pa·s	Basic

# Fluid 2

- I In the Model Builder window, right-click Materials and choose Blank Material.
- 2 Right-click Material 2 (mat2) and choose Rename.
- 3 In the Rename Material dialog box, type Fluid 2 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	1e3[kg/m^3]	kg/m³	Basic
Dynamic viscosity	mu	6.71e-3[Pa*s]	Pa∙s	Basic

#### DEFINITIONS

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 1e-3.
- 4 Click to expand the Smoothing section. In the Size of transition zone text field, type 2e-3.

Integration 1 (intop1)

Add a nonlocal integration coupling that you will use to calculate the effective droplet diameter according to Equation 1 in the **Model Definition** section.

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

Variables 1

- I In the **Definitions** toolbar, click  $\partial =$  **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
V1	0.4e-6/3600*step1(t[1/ s])[m^3/s]	m³/s	Volume flow, inlet 1
V2	0.2e-6/3600*step1(t[1/ s])[m^3/s]	m³/s	Volume flow, inlet 2
d_eff	2*(intop1((phils>0.5)* (x<-0.2[mm]))*3/(4* pi))^(1/3)	m	Effective droplet diameter

#### MULTIPHYSICS

Two-Phase Flow, Level Set 1 (tpf1)

- I In the Model Builder window, under Component I (compl)>Multiphysics click Two-Phase Flow, Level Set I (tpfl).
- 2 In the Settings window for Two-Phase Flow, Level Set, locate the Fluid I Properties section.
- 3 From the Fluid I list, choose Fluid I (matl).
- 4 Locate the Fluid 2 Properties section. From the Fluid 2 list, choose Fluid 2 (mat2).
- 5 Locate the Surface Tension section. Select the

Include surface tension force in momentum equation check box.

6 From the Surface tension coefficient list, choose User defined. In the  $\sigma$  text field, type 5e-3[N/m].

### LEVEL SET (LS)

Level Set Model I

- I In the Model Builder window, under Component I (compl)>Level Set (Is) click Level Set Model I.
- 2 In the Settings window for Level Set Model, locate the Level Set Model section.
- **3** In the  $\gamma$  text field, type 0.1[m/s].
- 4 In the  $\varepsilon_{ls}$  text field, type 5e-6.

#### MULTIPHYSICS

Wetted Wall I (wwI)

I In the Physics toolbar, click And Multiphysics Couplings and choose Boundary> Wetted Wall.

- **2** Select Boundaries 2–4, 6, 7, 9, 10, and 16–20 only.
- 3 In the Settings window for Wetted Wall, locate the Wetted Wall section.
- **4** From the **Slip length** list, choose **User defined**. In the  $\beta$  text field, type **5e-6**[m].
- **5** In the  $\theta_w$  text field, type 3\*pi/4[rad].

# LEVEL SET (LS)

Initial Values, Fluid 2 1

- I In the Model Builder window, under Component I (compl)>Level Set (Is) click Initial Values, Fluid 2 I.
- 2 Select Domain 3 only.

For Domains 1, 2 and 4, the default initial value settings apply.

# LAMINAR FLOW (SPF)

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

Inlet 1

- I In the Physics toolbar, click 🔚 Boundaries and choose Inlet.
- **2** Select Boundary 22 only.
- 3 In the Settings window for Inlet, locate the Boundary Condition section.
- **4** From the list, choose **Fully developed flow**.
- 5 Locate the Fully Developed Flow section. Click the Flow rate button.
- **6** In the  $V_0$  text field, type V1.

# Inlet 2

- I In the Physics toolbar, click 📄 Boundaries and choose Inlet.
- 2 Select Boundary 12 only.
- 3 In the Settings window for Inlet, locate the Boundary Condition section.
- 4 From the list, choose Fully developed flow.
- 5 Locate the Fully Developed Flow section. Click the Flow rate button.
- **6** In the  $V_0$  text field, type V2.

# Outlet I

- I In the Physics toolbar, click 🔚 Boundaries and choose Outlet.
- 2 Select Boundary 1 only.

Symmetry I

- I In the Physics toolbar, click 🔚 Boundaries and choose Symmetry.
- 2 Select Boundaries 5, 13, 14, and 21 only.

# LEVEL SET (LS)

In the Model Builder window, under Component I (compl) click Level Set (Is).

## Inlet 1

- I In the Physics toolbar, click 🔚 Boundaries and choose Inlet.
- **2** Select Boundary 12 only.
- 3 In the Settings window for Inlet, locate the Level Set Condition section.
- **4** From the list, choose **Fluid 2** ( $\phi$  = **I**).

# Inlet 2

- I In the Physics toolbar, click 📄 Boundaries and choose Inlet.
- **2** Click the 4 **Zoom Extents** button in the **Graphics** toolbar.
- **3** Select Boundary 22 only.

# Outlet I

- I In the Physics toolbar, click 🔚 Boundaries and choose Outlet.
- 2 Select Boundary 1 only.

#### Symmetry I

- I In the Physics toolbar, click 🔚 Boundaries and choose Symmetry.
- 2 Select Boundaries 5, 13, 14, and 21 only.

## MESH I

## Mapped I

- I In the Model Builder window, under Component I (comp1) right-click Mesh I and choose More Operations>Mapped.
- **2** Select Boundaries 2, 7, 10, and 16 only.

# Distribution I

- I Right-click Mapped I and choose Distribution.
- **2** Select Edge 3 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 In the Number of elements text field, type 160.

# Distribution 2

- I In the Model Builder window, right-click Mapped I and choose Distribution.
- 2 Select Edges 1 and 9 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 In the Number of elements text field, type 20.

# Distribution 3

- I Right-click Mapped I and choose Distribution.
- **2** Select Edges 12 and 28 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the Number of elements text field, type 25.
- 6 In the **Element ratio** text field, type 4.

#### Distribution 4

- I Right-click Mapped I and choose Distribution.
- **2** Select Edges 24 and 27 only.
- 3 In the Settings window for Distribution, locate the Distribution section.
- 4 From the **Distribution type** list, choose **Predefined**.
- 5 In the Number of elements text field, type 20.
- 6 In the **Element ratio** text field, type 3.
- 7 Select the **Reverse direction** check box.

#### Mapped I

Right-click Mapped I and choose Build Selected.

Swept I

- I In the Model Builder window, right-click Mesh I and choose Swept.
- 2 In the Settings window for Swept, click to expand the Source Faces section.
- **3** Select Boundaries 2, 7, and 10 only.

#### Distribution I

- I Right-click Swept I and choose Distribution.
- 2 In the Settings window for Distribution, locate the Distribution section.
- **3** In the Number of elements text field, type 10.

#### 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(0,2.5e-3,0.08).
- 4 Click to expand the Results While Solving section. Select the Plot check box.

This choice means that the **Graphics** window will show a surface plot of the volume fraction of **Fluid I** while solving, and this plot will be updated at each output time step.

# Solution 1 (soll)

Manually tune the solver sequence for optimal performance and accuracy.

- I In the Study toolbar, click **Show Default Solver**.
- 2 In the Model Builder window, expand the Solution I (soll) node.
- 3 In the Model Builder window, expand the Study I>Solver Configurations> Solution I (solI)>Dependent Variables 2 node, then click Velocity field (compl.u).
- 4 In the Settings window for Field, locate the Scaling section.
- 5 From the Method list, choose Manual.
- 6 In the Scale text field, type 0.1.

- 7 In the Model Builder window, click Time-Dependent Solver I.
- 8 In the Settings window for Time-Dependent Solver, click to expand the Time Stepping section.
- 9 From the Method list, choose Generalized alpha.
- **IO** From the **Steps taken by solver** list, choose **Manual**.
- II In the Time step text field, type 6.5e-5.
- 12 Find the Algebraic variable settings subsection. In theFraction of initial step for Backward Euler text field, type 1.
- **I3** In the **Study** toolbar, click **= Compute**.

# RESULTS

Velocity (spf)

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

#### Isosurface I

- I Right-click Velocity (spf) and choose Isosurface.
- 2 In the Settings window for Isosurface, locate the Expression section.
- **3** In the **Expression** text field, type 1s.Vf1.
- 4 Locate the Levels section. From the Entry method list, choose Levels.
- 5 In the Levels text field, type 0.5.
- 6 Locate the Coloring and Style section. From the Coloring list, choose Uniform.
- 7 From the Color list, choose Gray.
- 8 In the Velocity (spf) toolbar, click **O** Plot.

#### Volume Fraction

- I In the Model Builder window, click Pressure (spf).
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Dataset list, choose Study I/Solution I (soll).
- 4 Right-click Pressure (spf) and choose Rename.
- 5 In the **Rename 3D Plot Group** dialog box, type Volume Fraction in the **New label** text field.
- 6 Click OK.

Slice 1

I Right-click Volume Fraction and choose Slice.

2 In the Settings window for Slice, locate the Expression section.

3 In the **Expression** text field, type 1s.Vf1.

## Pressure

In the Model Builder window, right-click Pressure and choose Delete.

## Surface

In the Model Builder window, right-click Surface and choose Delete.

# Volume Fraction of Fluid 1 (Is)

Now, the first default plot group shows a slice plot of the velocity combined with a contour plot of the volume fraction of fluid 1, and the second plot group shows the volume fraction of fluid 1 as a slice plot. Follow these steps to reproduce the series of velocity field plots shown in Figure 3.

# Slice 1

- I In the Model Builder window, expand the Volume Fraction of Fluid I (Is) node.
- 2 Right-click Slice I and choose Disable.

#### Isosurface 1

- I In the Model Builder window, click Isosurface I.
- 2 In the Settings window for Isosurface, locate the Coloring and Style section.
- 3 From the Color list, choose White.

#### Isosurface 2

Right-click Results>Volume Fraction of Fluid I (Is)>Isosurface I and choose Duplicate.

#### Deformation I

- I In the Model Builder window, right-click Isosurface 2 and choose Deformation.
- 2 In the Settings window for Deformation, locate the Expression section.
- **3** In the **y** component text field, type -2\*y.
- 4 Locate the Scale section. Select the Scale factor check box.
- **5** In the associated text field, type **1**.

#### Streamline 1

- I In the Model Builder window, right-click Volume Fraction of Fluid I (Is) and choose Streamline.
- 2 In the Settings window for Streamline, locate the Streamline Positioning section.
- 3 In the Number text field, type 8.

- **4** Select Boundaries 12 and 22 only.
- 5 Locate the Coloring and Style section. Find the Line style subsection. From the Type list, choose Tube.
- 6 Select the Radius scale factor check box.
- 7 In the associated text field, type 2e-3.

#### Color Expression 1

- I Right-click Streamline I and choose Color Expression.
- 2 In the Settings window for Color Expression, locate the Coloring and Style section.
- 3 From the Color table list, choose JupiterAuroraBorealis.
- 4 Clear the Color legend check box.

# Streamline 2

In the Model Builder window, under Results>Volume Fraction of Fluid I (Is) right-click Streamline I and choose Duplicate.

## Deformation I

- I In the Model Builder window, right-click Streamline 2 and choose Deformation.
- 2 In the Settings window for Deformation, locate the Expression section.
- **3** In the **y** component text field, type -2\*y.
- **4** Locate the **Scale** section. Select the **Scale factor** check box.
- **5** In the associated text field, type **1**.

#### Surface 1

- I In the Model Builder window, right-click Volume Fraction of Fluid I (Is) and choose Surface.
- 2 In the Settings window for Surface, locate the Coloring and Style section.
- **3** From the **Coloring** list, choose **Uniform**.
- 4 From the Color list, choose Gray.

## Selection I

- I Right-click Surface I and choose Selection.
- 2 Select Boundaries 3 and 17–20 only.

## Surface 2

In the Model Builder window, under Results>Volume Fraction of Fluid I (Is) right-click Surface I and choose Duplicate.

## Deformation I

- I In the Model Builder window, expand the Surface 2 node.
- 2 Right-click Surface 2 and choose Deformation.
- 3 In the Settings window for Deformation, locate the Expression section.
- **4** In the **y** component text field, type 0.05.
- **5** Locate the **Scale** section. Select the **Scale factor** check box.
- 6 In the associated text field, type 1.

Selection 1

- I In the Model Builder window, click Selection I.
- 2 In the Settings window for Selection, locate the Selection section.
- **3** Select the **Image Activate Selection** toggle button.
- 4 Select Boundaries 3–6, 9, 13, 14, and 17–21 only.

Volume Fraction of Fluid 1 (ls)

- I In the Model Builder window, click Volume Fraction of Fluid I (Is).
- 2 In the Settings window for 3D Plot Group, locate the Data section.
- 3 From the Time (s) list, choose 0.02.
- 4 Locate the Plot Settings section. Clear the Plot dataset edges check box.
- 5 In the Volume Fraction of Fluid I (Is) toolbar, click 🗿 Plot.
- 6 Click 🗿 Plot.



Compare the resulting plot with the upper-left plot in Figure 3.To reproduce the remaining three plots, plot the solution for the time values 0.04, 0.06, and 0.08 s.

Global Evaluation 1

Next, evaluate the effective droplet diameter computed according to Equation 1.

- I In the Results toolbar, click (8.5) Global Evaluation.
- 2 In the Settings window for Global Evaluation, click Replace Expression in the upper-right corner of the Expressions section. From the menu, choose Component I (compl)> Definitions>Variables>d\_eff Effective droplet diameter m.
- 3 Click **=** Evaluate.

# TABLE

I Go to the Table window.

The result, roughly 0.12 mm, is displayed in the table in the **Table** window.

# RESULTS

Finally, generate a movie of the moving fluid interface and the velocity streamlines.

Volume Fraction of Fluid 1 (ls)

In the Model Builder window, under Results click Volume Fraction of Fluid I (Is).

# Animation I

I In the Volume Fraction of Fluid I (Is) toolbar, click Animation and choose Player. COMSOL Multiphysics generates the movie. To play the movie, click the Play button in the Graphics toolbar. If you want to export a movie in GIF, Flash, or AVI format, select File from the Target list.

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