



Model created in COMSOL Multiphysics 6.4

# Bubble-Induced Entrainment Between Stratified Liquid Layers

## Introduction

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Three-phase flows occur in numerous industrial applications, in free and porous media (nuclear safety, petroleum engineering, and so on). Many biomedical and chemical processes involve mixtures of three or more fluids, for example double emulsions, which play critical roles in applications such as prolonged drug delivery systems, entrapment of vitamins and flavor encapsulation for food additives. Considering a configuration of two immiscible liquids in stratified layers, it is known that a gas bubble of sufficient size rising through the stratified layers can entrain some of the heavier liquid from the lower layer into its wake and transport it to the upper layer of lighter liquid. This entrainment phenomenon has significant effects on both heat and mass transfer, and is encountered in a number of industrial applications. For example, in chemical processing, gas bubbles are sometimes released into pools of stratified liquids to induce mixing and phase transport. In nuclear-reactor safety applications, bubbles of noncondensable gas rise through stratified liquid pools of molten fuel and materials. In metallurgical processing, bubbles of oxygen and other gases may bubble through pools of molten metal with overlying pools of molten silica slag (Ref. 1).

However, computational models for direct simulation of three-phase flow are rather rare in comparison with the large body of research on two-phase flow. The current model, based on the predefined multiphysics coupling between the Laminar Flow and Ternary Phase Field interfaces, simulates three-phase flow (gas and two liquids) with large density and viscosity differences.

This benchmark model simulates a single gas bubble which rises through the interface between two stratified liquid layers thereby inducing entrainment, and validates the results against literature (Ref. 2).

## Model Setup

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When a gas bubble rises in a two-stratified-liquid-layers configuration, the bubble can either become captured at the interface, or penetrate into the light phase, possibly leading to entrainment of the heavy phase. The criterion is based on a macroscopic balance between buoyancy and surface tension forces, and states that the bubble will penetrate the liquid-liquid interface, if its volume,  $V$ , satisfies (Ref. 2),

$$V > V^c = \left( \frac{2\pi \left(\frac{3}{4\pi}\right)^{1/3} \sigma_{23}}{(\rho_3 - \rho_1)g} \right)^{\frac{3}{2}}$$

where  $g$  denotes the gravity constant,  $\sigma$  denotes the surface tension, and 1, 2, 3 are the suffixes for gas, heavy liquid, and light liquid, respectively. This criterion has been validated both experimentally and numerically (Ref. 1, Ref. 2).

This model is one of the case considered in Ref. 2. The physical properties of the fluids used in the simulation are listed in Table 1 and Table 2.

TABLE 1: SURFACE TENSION BETWEEN THREE PHASES.

Parameters	Surface tension (N/m)
$\sigma_{12}, \sigma_{13}$ (between the gas and the two liquids)	0.07
$\sigma_{23}$ (between the two liquids)	0.05

TABLE 2: PHYSICAL PROPERTIES OF THREE PHASES.

	Density ( $\text{kg/m}^3$ )	Viscosity (Pa·s)
Bubble	1	1e-4
Heavy liquid	1200	0.15
Light liquid	1000	0.1

Inserting the physical parameters above in Equation gives  $V^c = 8.8726 \cdot 10^{-8} \text{ kg/m}^3$ . Because the volume of a sphere is given by  $V = 4\pi r^3/3$ , the critical bubble radius can be estimated to be  $r^c = 2.778 \text{ mm}$ .

The radius of the bubble in the simulation is  $r = 8 \text{ mm}$ . Since  $r > r^c$ , the gas bubble will penetrate the liquid-liquid interface. Due to its relatively large volume, it will furthermore entrain some of the heavy liquid into its wake and transport it into the light liquid forming small droplets of heavy liquid in the upper layer. The mobility  $M_0$ , which is taken as a function of the phase field variables, is defined in such a way that it becomes zero in each pure phase,  $M_0 = M_{\text{const}}(\phi_A^2 \phi_B^2 + \phi_A^2 \phi_C^2 + \phi_B^2 \phi_C^2)$ , where  $M_{\text{const}} = 2 \cdot 10^{-5} \text{ m}^3/\text{s}$ .

The model is axisymmetric; [Figure 1](#) shows its geometry. The mesh contains around 36150 elements with linear shape functions. The simulation time interval is between 0 and 0.65 s, which is around the time the bubble needs to rise through the given column.

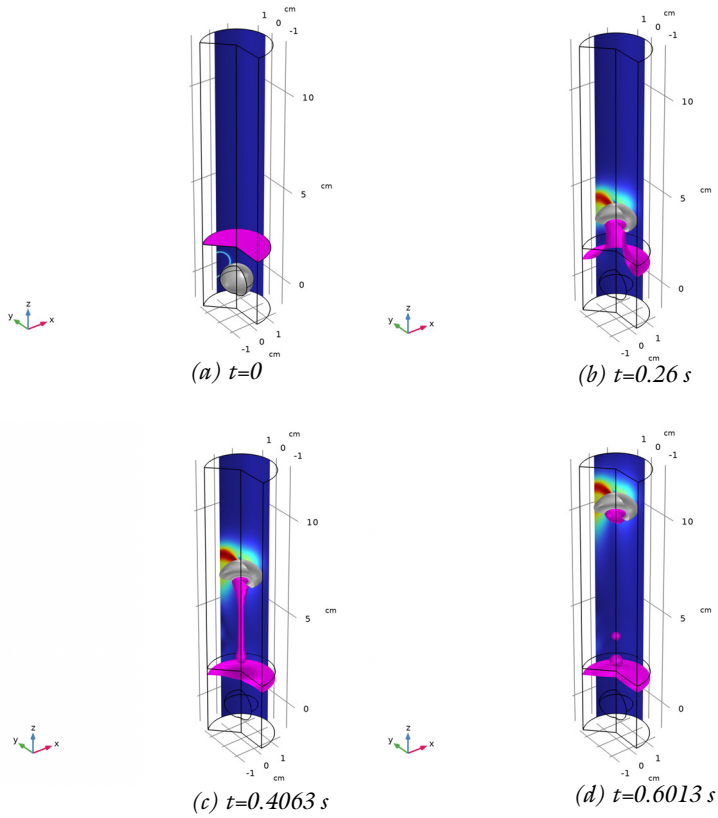


*Figure 1: Geometry of the computation domain.*

### *Results and Discussion*

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The simulation results are shown in [Figure 2](#). Initially, a gas bubble is placed underneath the surface between a heavy liquid and a light liquid, see [Figure 2\(a\)](#). The gas bubble then passes into the upper pool and a volume of heavy liquid is clearly seen to be entrained in its wake, having been pulled through the interfaces between the two liquid layers, see [Figure 2\(b\)](#). If the bubble were of insufficient size, the levitated column would fall back to the lower pool and the gas bubble would continue to rise through the upper pool without having caused any entrainment. This is not the case in current model. Here, the size of the bubble is sufficiently large that the levitated liquid column rises to a height such that it eventually pinches off from the lower layer, see [Figure 2\(c\)](#). As the column elongates, it becomes hydro-dynamically unstable and pinches off into a series of small droplets. A small amount of the heavy liquid adheres to the bubble, see [Figure 2\(d\)](#), and can be considered to have been successfully entrained into the upper fluid layer.



*Figure 2: Processing of bubble-induced entrainment between stratified liquid layers. The silver and pink surfaces represent the interfaces between gas and light liquid and between light liquid and heavy liquid, respectively. The colored surface half-enclosing the domain represents the velocity field magnitude.*

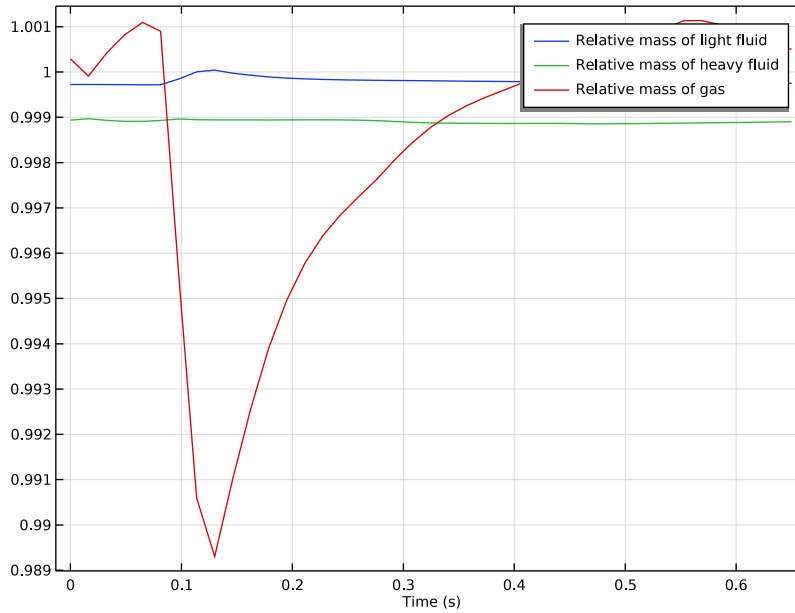


Figure 3: History of mass changes.

It is important that the mass of each phase is conserved to within a tolerance given by the numerical method and the computational mesh. The mass conservation history is shown in Figure 3. It is observed that the mass loss for the two liquid phases is about 0.1%, and that of the gas phase is about 1.5%. The mass loss of gas is the largest because its volume fraction is much smaller than the other two phases, whereby its relative change becomes most noticeable.

## References

1. G.A. Green, J.C. Chen, and M.T. Conlin, "Bubble induced entrainment between stratified liquid layers," *International Journal of Heat and Mass Transfer*, vol. 34, pp 149–157, 1991.
2. F. Boyer, C. Lapuerta, S. Minjeaud, B. Piar, and M. Quintard, "Cahn-Hilliard/Navier-Stokes Model for the Simulation of Three-Phase Flows," *Transport in Porous Media*, vol. 82, pp 463–483, 2010.

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**Application Library path:** Microfluidics\_Module/Three-Phase\_Flow/  
three\_phase\_bubble

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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 **Fluid Flow** > **Multiphase Flow** > **Three-Phase Flow, Phase Field** > **Laminar Three-Phase Flow, Phase Field**.
- 3 Click **Add**.
- 4 Click  **Study**.
- 5 In the **Select Study** tree, select **General Studies** > **Time Dependent**.
- 6 Click  **Done**.

#### **GEOMETRY I**

- 1 In the **Model Builder** window, under **Component I (comp1)** click **Geometry I**.
- 2 In the **Settings** window for **Geometry**, locate the **Units** section.
- 3 From the **Length unit** list, choose **cm**.


#### **GLOBAL DEFINITIONS**

##### *Parameters I*

- 1 In the **Model Builder** window, under **Global Definitions** click **Parameters I**.
- 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 `three_phase_bubble_parameters.txt`.

## DEFINITIONS

### *Variables 1*


- 1 In the **Model Builder** window, under **Component 1 (comp1)** right-click **Definitions** and choose **Variables**.
- 2 In the **Settings** window for **Variables**, locate the **Variables** section.
- 3 Click  **Load from File**.
- 4 Browse to the model's Application Libraries folder and double-click the file `three_phase_bubble_variables.txt`.

## GEOMETRY 1

### *Rectangle 1 (r1)*

- 1 In the **Model Builder** window, expand the **Component 1 (comp1)** > **Geometry 1** node.
- 2 Right-click **Geometry 1** and choose **Rectangle**.
- 3 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.
- 4 In the **Width** text field, type `width/2`.
- 5 In the **Height** text field, type `height`.
- 6 Locate the **Position** section. From the **Base** list, choose **Center**.
- 7 In the **r** text field, type `width/4`.
- 8 In the **z** text field, type `center_rec`.

### *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 `radius`.
- 4 In the **Sector angle** text field, type `180`.
- 5 Locate the **Position** section. In the **z** text field, type `center_bub`.
- 6 Locate the **Rotation Angle** section. In the **Rotation** text field, type `-90`.


### *Polygon 1 (pol1)*

- 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:

r (cm)	z (cm)
0	line_z
radius*2	line_z

*Form Union (fin)*


In the **Geometry** toolbar, click  **Build All**.

## TERNARY PHASE FIELD (TERPF)

*Mixture Properties 1*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Ternary Phase Field (terpf)** click **Mixture Properties 1**.
- 2 In the **Settings** window for **Mixture Properties**, locate the **Phase Field Parameters** section.
- 3 In the  $M_0$  text field, type M0.
- 4 Locate the **Surface Tension** section. From the **Surface tension coefficient of interface between phase A and phase B** list, choose **User defined**. In the  $\sigma_{A,B}$  text field, type sigma\_AB.
- 5 From the **Surface tension coefficient of interface between phase B and phase C** list, choose **User defined**. In the  $\sigma_{B,C}$  text field, type sigma\_BC.
- 6 From the **Surface tension coefficient of interface between phase A and phase C** list, choose **User defined**. In the  $\sigma_{A,C}$  text field, type sigma\_AC.

*Initial Values 2*

- 1 In the **Physics** toolbar, click  **Domains** and choose **Initial Values**.
- 2 Select Domain 1 only.
- 3 In the **Settings** window for **Initial Values**, locate the **Initial Values** section.
- 4 In the  $\phi_{iB}$  text field, type 1.

*Initial Values 3*


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

*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  $\phi_{iA}$  text field, type 1.

## MULTIPHYSICS

### *Three-Phase Flow, Phase Field 1 (tppf1)*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Multiphysics** click **Three-Phase Flow, Phase Field 1 (tppf1)**.
- 2 In the **Settings** window for **Three-Phase Flow, Phase Field**, locate the **Material Properties** section.
- 3 Click  **Add Multiphase Material**.

## MATERIALS

### *Fluid A*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Materials > Multiphase Material 1 (mpmat1)** click **Phase 1 (mpmat1.phase1)**.
- 2 In the **Settings** window for **Phase**, locate the **Material Contents** section.
- 3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rho_A	kg/m <sup>3</sup>	Basic
Dynamic viscosity	mu	mu_A	Pa·s	Basic

- 4 In the **Label** text field, type Fluid A.

### *Fluid B*

- 1 In the **Model Builder** window, under **Component 1 (comp1) > Materials > Multiphase Material 1 (mpmat1)** click **Phase 2 (mpmat1.phase2)**.
- 2 In the **Settings** window for **Phase**, type Fluid B in the **Label** text field.
- 3 Locate the **Material Contents** section. In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rho_B	kg/m <sup>3</sup>	Basic
Dynamic viscosity	mu	mu_B	Pa·s	Basic

### *Fluid C*

- 1 In the **Model Builder** window, click **Phase 3 (mpmat1.phase3)**.
- 2 In the **Settings** window for **Phase**, locate the **Material Contents** section.



3 In the table, enter the following settings:

Property	Variable	Value	Unit	Property group
Density	rho	rho_C	kg/m <sup>3</sup>	Basic
Dynamic viscosity	mu	mu_C	Pa·s	Basic

4 In the **Label** text field, type Fluid C.

## DEFINITIONS

### Ramp 1 (rm1)

- 1 In the **Definitions** toolbar, click  **More Functions** and choose **Ramp**.
- 2 In the **Settings** window for **Ramp**, locate the **Parameters** section.
- 3 In the **Slope** text field, type 200.
- 4 Select the **Cutoff** checkbox.
- 5 Click  **Plot**.

## LAMINAR FLOW (SPF)


- 1 In the **Model Builder** window, under **Component 1 (comp1)** click **Laminar Flow (spf)**.
- 2 In the **Settings** window for **Laminar Flow**, locate the **Physical Model** section.
- 3 Select the **Include gravity** checkbox.

### Gravity 1

- 1 In the **Model Builder** window, under **Component 1 (comp1)** > **Laminar Flow (spf)** click **Gravity 1**.
- 2 In the **Settings** window for **Gravity**, locate the **Acceleration of Gravity** section.
- 3 Specify the **g** vector as

0	r
-g_const*rm1(t[1/s])	z

### Pressure Point Constraint 1


- 1 In the **Physics** toolbar, click  **Points** and choose **Pressure Point Constraint**.
- 2 Select Point 8 only.

## 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 Click the **Custom** button.
- 4 Locate the **Element Size Parameters** section. In the **Maximum element size** text field, type 0.04.
- 5 Click  **Build All**.

### STUDY 1

#### Step 1: Time Dependent

- 1 In the **Model Builder** window, under **Study 1** click **Step 1: Time Dependent**.
- 2 In the **Settings** window for **Time Dependent**, locate the **Study Settings** section.
- 3 In the **Output times** text field, type range (0, 0.025, 1) \* 0.65.

#### Solution 1 (sol1)

In the **Study** toolbar, click  **Show Default Solver**.

#### 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**, click to expand the **Results While Solving** section.
- 3 Select the **Plot** checkbox.
- 4 From the **Update at** list, choose **Time steps taken by solver**.

#### Solution 1 (sol1)

- 1 In the **Model Builder** window, expand the **Study 1 > Solver Configurations > Solution 1 (sol1)** node, then click **Time-Dependent Solver 1**.
- 2 In the **Settings** window for **Time-Dependent Solver**, click to expand the **Time Stepping** section.
- 3 From the **Maximum step constraint** list, choose **Constant**.
- 4 In the **Maximum step** text field, type 0.0005.

### RESULTS

- 1 In the **Model Builder** window, expand the **Results** node.


- 2 Right-click **Study 1** > **Solver Configurations** > **Solution 1 (sol1)** > **Time-Dependent Solver 1** and choose **Get Initial Value**.

## STUDY 1

### *Step 1: Time Dependent*


- 1 In the **Settings** window for **Time Dependent**, locate the **Results While Solving** section.
- 2 In the table, enter the following settings:

Plot group	Plot window
2D Plot Group: Three Phases (terpf)	Graphics

- 3 In the **Study** toolbar, click  **Compute**.

## RESULTS

### *3D Plot Group 8*


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

### *Isosurface 1*

- 1 Right-click **3D Plot Group 8** and choose **Isosurface**.
- 2 In the **Settings** window for **Isosurface**, locate the **Expression** section.
- 3 In the **Expression** text field, type  $\phi_B$ .
- 4 Locate the **Levels** section. From the **Entry method** list, choose **Levels**.
- 5 In the **Levels** text field, type 0.5.
- 6 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 7 Locate the **Coloring and Style** section. From the **Coloring** list, choose **Uniform**.
- 8 Clear the **Color legend** checkbox.
- 9 From the **Color** list, choose **Magenta**.

### *Isosurface 2*


- 1 In the **Model Builder** window, right-click **3D Plot Group 8** and choose **Isosurface**.
- 2 In the **Settings** window for **Isosurface**, locate the **Expression** section.
- 3 In the **Expression** text field, type  $\text{terpf}.\phi_C$ .
- 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 Locate the **Title** section. From the **Title type** list, choose **None**.
- 8 Locate the **Coloring and Style** section. Clear the **Color legend** checkbox.
- 9 From the **Color** list, choose **Gray**.
- 10 In the **3D Plot Group 8** toolbar, click  **Plot**.




#### *Slice 1*

- 1 Right-click **3D Plot Group 8** and choose **Slice**.
- 2 In the **Settings** window for **Slice**, locate the **Plane Data** section.
- 3 In the **Planes** text field, type 1.
- 4 From the **Plane** list, choose **zx-planes**.
- 5 In the **Planes** text field, type 1.


#### *Deformation 1*

- 1 Right-click **Slice 1** and choose **Deformation**.
- 2 In the **Settings** window for **Deformation**, locate the **Expression** section.
- 3 From the **Coordinate system** list, choose **Global Cartesian**.
- 4 In the **x-component** text field, type 0.
- 5 In the **y-component** text field, type  $\sqrt{0.016^2 - r^2}$ .
- 6 In the **z-component** text field, type 0.
- 7 Locate the **Scale** section.
- 8 Select the **Scale factor** checkbox. In the associated text field, type 1.
- 9 In the **3D Plot Group 8** toolbar, click  **Plot**.

#### *3D Plot Group 8*

- 1 In the **Model Builder** window, under **Results** click **3D Plot Group 8**.
- 2 In the **Settings** window for **3D Plot Group**, locate the **Data** section.
- 3 From the **Time (s)** list, choose **0**.
- 4 Locate the **Color Legend** section. Clear the **Show legends** checkbox.
- 5 Click to expand the **Title** section. From the **Title type** list, choose **None**.
- 6 In the **3D Plot Group 8** toolbar, click  **Plot**.
- 7 Locate the **Data** section. From the **Time (s)** list, choose **0.21125**.
- 8 In the **3D Plot Group 8** toolbar, click  **Plot**.
- 9 From the **Time (s)** list, choose **0.40625**.
- 10 In the **3D Plot Group 8** toolbar, click  **Plot**.

11 From the **Time (s)** list, choose **0.60125**.

12 In the **3D Plot Group 8** toolbar, click  **Plot**.

### *Surface Integration 1*

1 In the **Results** toolbar, click  $8.85 \times 10^{-12}$  **More Derived Values** and choose **Integration > Surface Integration**.

Integrate the volume fractions over the whole domain and divide by the initial volume of each phase to see how well the different volumes are conserved during simulation.

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

3 From the **Selection** list, choose **All domains**.

4 Locate the **Expressions** section. In the table, enter the following settings:

Expression	Unit	Description
$\text{tfpf1.VfA}/8.447\text{E-}5[\text{m}^3]$	1	
$\text{tfpf1.VfB}/2.603\text{e-}5[\text{m}^3]$	1	
$\text{tfpf1.VfC}/2.1451\text{e-}6[\text{m}^3]$	1	

5 Click  **Evaluate**.

### **TABLE 1**

1 Go to the **Table 1** window.

2 Click the **Table Graph** button in the window toolbar.

### **RESULTS**

#### *Table Graph 1*

1 In the **Settings** window for **Table Graph**, click to expand the **Legends** section.

2 Select the **Show legends** checkbox.

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

4 In the table, enter the following settings:

Legends
Relative mass of light fluid
Relative mass of heavy fluid
Relative mass of gas