Phase Separation

Introduction

Phase separation occurs when a binary system is quenched from a stable, homogeneous one-phase state into the two-phase region of its phase diagram. The spontaneous separation of two immiscible fluids is sometimes referred to as *spinodal decomposition*. Each phase tends to separate into pure components. This model demonstrates how to use the Phase Field interface to model the process of phase separation, see Ref. 1 for more information.

Model Definition

This simple benchmark model takes two initially mixed, immiscible phases and observes their separation into pure components. The components are represented by a phase field function, ϕ, and are considered pure when $\phi = \pm 1$. The initial mixture is created by putting ϕ equal to a random number with zero mean and a standard deviation of 0.05. The initial random perturbation initiates the separation into pure phases.

The separation of the two immiscible phases is described by the Cahn-Hilliard equation:

$$\frac{\partial \phi}{\partial t} = \nabla \cdot \frac{\gamma \lambda}{\varepsilon^2} \nabla \psi \tag{1}$$

where ϕ is the dimensionless phase field variable, so that the volume fractions of the components of the fluid are $(1+\phi)/2$ and $(1-\phi)/2$. The variable γ is the mobility ($\mathrm{m}^3 \cdot \mathrm{s/kg}$), the quantity λ is the mixing energy density (N), and ε is a capillary width that scales with the thickness of the interface (m). The latter two parameters are related to the surface tension coefficient through the equation

$$\sigma = \frac{2\sqrt{2}}{3} \frac{\lambda}{\varepsilon} \tag{2}$$

The equation governing ψ is

$$\psi = -\nabla \cdot \varepsilon^2 \nabla \phi + (\phi^2 - 1)\phi \tag{3}$$

BOUNDARY CONDITIONS

A contact angle is imposed on the boundaries. Mathematically, the boundary condition is

$$\mathbf{n} \cdot \varepsilon^2 \nabla\phi = \varepsilon^2 \tan(\pi/2 - \theta_w)|\nabla\phi - (\mathbf{n} \cdot \nabla\phi)\mathbf{n}| \quad (4)$$

and

$$\mathbf{n} \cdot \frac{\gamma\lambda}{\varepsilon^2}\nabla\psi = 0 \quad (5)$$

In COMSOL Multiphysics, the only input required is a contact angle, θ_w. The total mass in the system is computed by integrating the phase field variable over the domain:

$$\phi_{int} = \int \phi \, dV \quad (6)$$

This integrated quantity should remain constant during the separation of the two phases.

Results and Discussion

Figure 1 shows the evolution of the phase field variable. Initially, the two phases are completely mixed except for a random perturbation around $\phi = 0$. By $t = 1$ s the phases have started to separate. At $t = 2$ s, pure phases have started to form, and two seconds later only pure phases exist. After $t = 4$ s, the pure phases begin to coalesce to form large phase domains.

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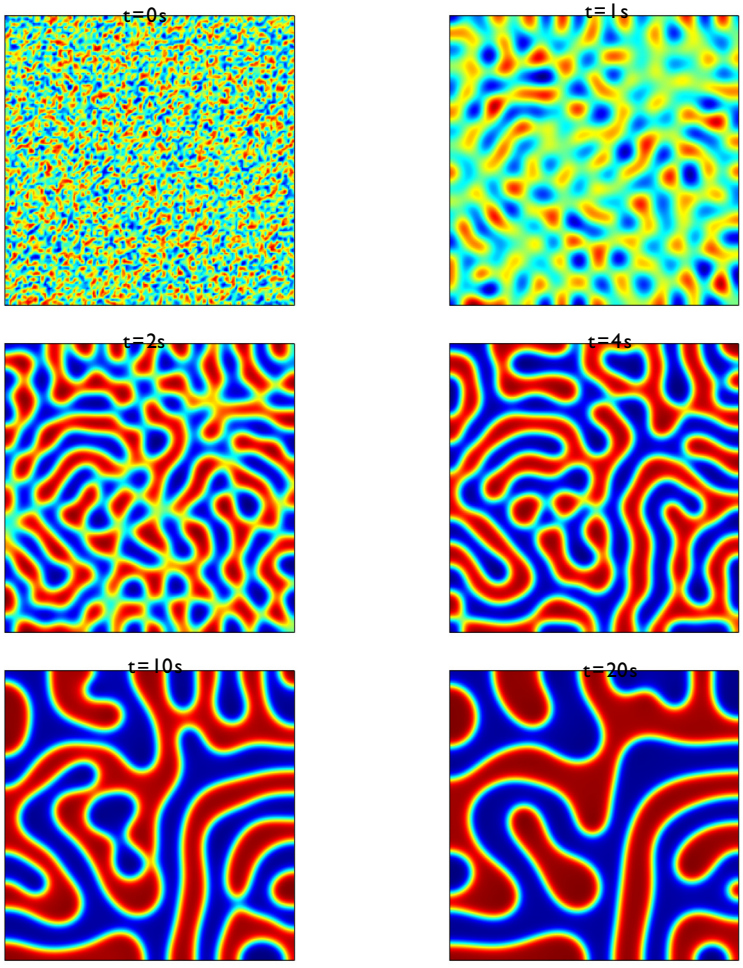

Figure 1: Plot of phase field variable at different time steps. The two fluids tend to separate into distinct phases. Blue represents $\phi = -1$, *red represents* $\phi = 1$, *and green represents* $\phi = 0$.

The Cahn-Hilliard equation is a mass conservation law, and it is possible to compute and visualize the degree to which mass is conserved. This is done by plotting the total mass in the system versus time, which is computed using Equation 6. Figure 2 plots this quantity versus time. The plot shows that the numerical model conserves the total mass in the system perfectly.

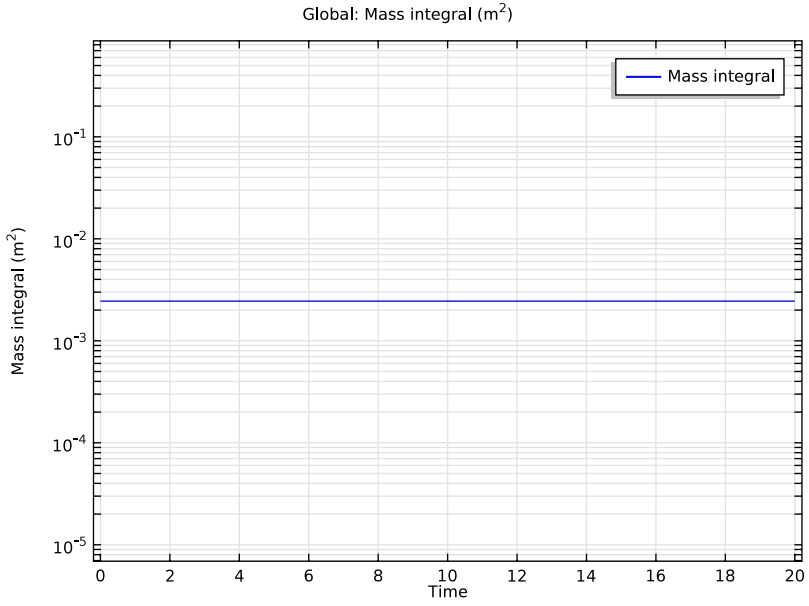

Figure 2: Plot of phase field variable integrated over the volume as a function of time. The total amount of mass in the system is perfectly conserved.

Reference

1. P. Zhang, *Periodic Phase Separation: A Numerical Study via a Modified Cahn-Hilliard Equation*, M.Sc. thesis, Dept. of Mathematics, Simon Fraser University, 2006.

Model Library path: `CFD_Module/Multiphase_Tutorials/phase_separation`

Modeling Instructions

MODEL WIZARD

1 Go to the **Model Wizard** window.

2 Click the **2D** button.

3 Click **Next**.

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4 In the **Add physics** tree, select **Mathematics>Moving Interface>Phase Field (pf)**.

5 Click **Add Selected**.

6 Click **Next**.

7 Find the **Studies** subsection. In the tree, select **Preset Studies>Time Dependent**.

8 Click **Finish**.

GEOMETRY 1

Square 1

1 In the **Model Builder** window, under **Model 1** right-click **Geometry 1** and choose **Square**.

2 In the **Square** settings window, locate the **Size** section.

3 In the **Side length** edit field, type `2*pi`.

4 Click the **Build All** button.

GLOBAL DEFINITIONS

The following steps define `phi_init` as a function whose values are samples of uniformly distributed random variables in `[-0.05,0.05]`.

Random 1

1 In the **Model Builder** window, under **Global Definitions** click **Random 1**.

2 In the **Random** settings window, locate the **Function Name** section.

3 In the **Function name** edit field, type `phi_init`.

4 Locate the **Parameters** section. In the **Number of arguments** edit field, type `2`.

5 In the **Range** edit field, type `0.1`.

PHASE FIELD

Phase Field Model 1

1 In the **Model Builder** window, expand the **Phase Field** node, then click **Phase Field Model 1**.

2 In the **Phase Field Model** settings window, locate the **Phase Field Parameters** section.

3 In the ε_{pf} edit field, type `0.08`.

Initial Values 1

1 In the **Model Builder** window, under **Model 1>Phase Field** click **Initial Values 1**.

2 In the **Initial Values** settings window, locate the **Initial Values** section.

3 In the ϕ edit field, type `phi_init(x,y)`.

DEFINITIONS

Integration 1

1 In the **Model Builder** window, under **Model 1** right-click **Definitions** and choose **Model Couplings>Integration**.

2 Select Domain 1 only.

Variables 1

1 In the **Model Builder** window, right-click **Definitions** and choose **Variables**.

2 In the **Variables** settings window, locate the **Variables** section.

3 In the table, enter the following settings:

Name	Expression	Description
`phi_int`	`intop1(phipf)`	`Mass integral`

Later, you will use this integral to verify that the total amount of mass in the system is conserved.

MESH 1

In the **Model Builder** window, under **Model 1** right-click **Mesh 1** and choose **Mapped**.

Size

1 In the **Model Builder** window, under **Model 1>Mesh 1** click **Size**.

2 In the **Size** settings window, locate the **Element Size** section.

3 From the **Predefined** list, choose **Extra fine**.

4 Click the **Build All** button.

STUDY 1

Step 1: Time Dependent

1 In the **Model Builder** window, expand the **Study 1** node, then click **Step 1: Time Dependent**.

2 In the **Time Dependent** settings window, locate the **Study Settings** section.

3 In the **Times** edit field, type `range(0,0.5,20)`.

4 Click to expand the **Results While Solving** section. Select the **Plot** check box.

5 In the **Model Builder** window, right-click **Study 1** and choose **Compute**.

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RESULTS

2D Plot Group 1

1 In the **Model Builder** window, under **Results** click **2D Plot Group 1**.

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

3 From the **Time** list, choose **0**.

4 Locate the **Title** section. From the **Title type** list, choose **Manual**.

5 In the **Title** text area, type `t = 0 s`.

6 Click the **Plot** button.

7 Click the **Zoom Extents** button on the Graphics toolbar.

8 Locate the **Data** section. From the **Time** list, choose **1**.

9 Locate the **Title** section. In the **Title** text area, type `t = 1 s`.

10 Click the **Plot** button.

11 Locate the **Data** section. From the **Time** list, choose **2**.

12 Locate the **Title** section. In the **Title** text area, type `t = 2 s`.

13 Click the **Plot** button.

14 Locate the **Data** section. From the **Time** list, choose **4**.

15 Locate the **Title** section. In the **Title** text area, type `t = 4 s`.

16 Click the **Plot** button.

17 Locate the **Data** section. From the **Time** list, choose **10**.

18 Locate the **Title** section. In the **Title** text area, type `t = 10 s`.

19 Click the **Plot** button.

20 Locate the **Data** section. From the **Time** list, choose **20**.

21 Locate the **Title** section. In the **Title** text area, type `t = 20 s`.

22 Click the **Plot** button.

1D Plot Group 2

1 In the **Model Builder** window, right-click **Results** and choose **1D Plot Group**.

2 Right-click **1D Plot Group 2** and choose **Global**.

3 In the **Global** settings window, click **Replace Expression** in the upper-right corner of the **y-Axis Data** section. From the menu, choose **Definitions>Mass integral (phi_int)**.

4 Click the **y-Axis Log Scale** button on the Graphics toolbar.

5 Click the **Plot** button.

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6 Click the **Zoom Extents** button on the Graphics toolbar.

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