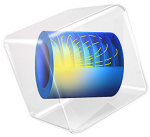

Phase Separation

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 example 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:

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

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

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

The equation governing ψ is

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

In the Phase Field interface, the volume fractions of the individual fluids are

$$V_{\mathrm{f1}} = \frac{1-\phi}{2}, \qquad V_{\mathrm{f2}} = \frac{1+\phi}{2}$$

The Wetted Wall default boundary condition is imposed on the boundary. Mathematically, the boundary condition is

$$\mathbf{n} \cdot \varepsilon^2 \nabla \phi = \varepsilon^2 \cos(\theta_w) |\nabla \phi|$$

and

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

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:

$$\phi_{int} = \int \phi \, dV \tag{1}$$

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

Results and Discussion

Figure 1 shows the evolution of the volume fraction V_{f1}. 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.

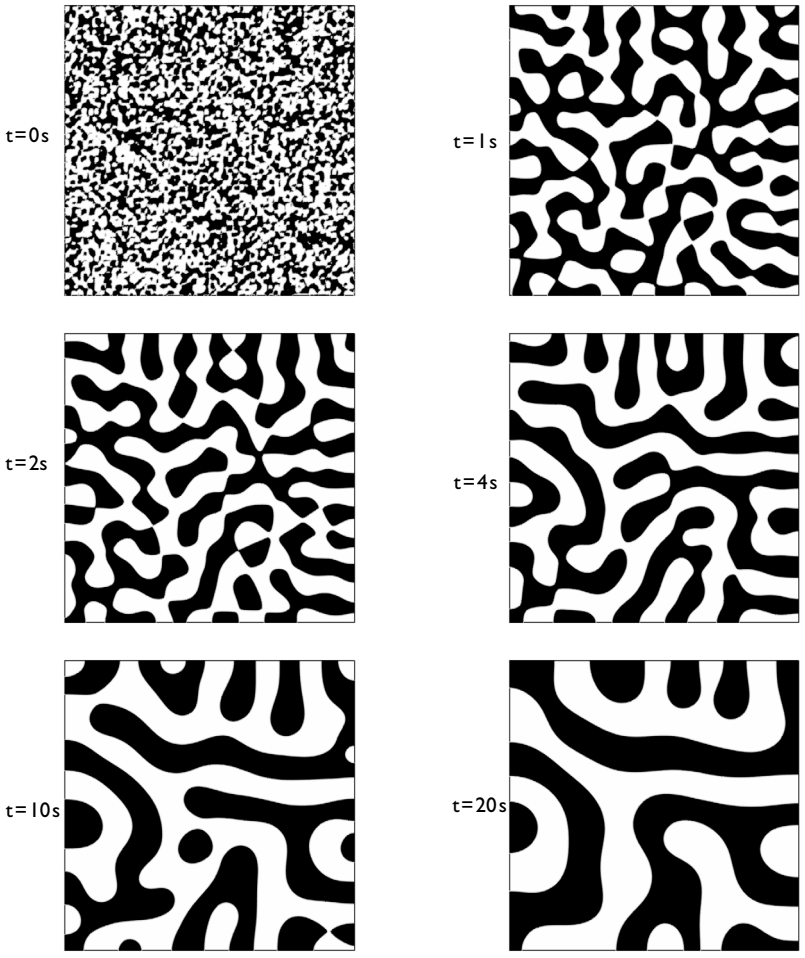

Figure 1: The two fluids tend to separate into distinct phases. Black represents fluid 1, white represents fluid 2.

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 1. Figure 2 plots this quantity versus time. The plot shows that the numerical model conserves the total mass in the system perfectly.

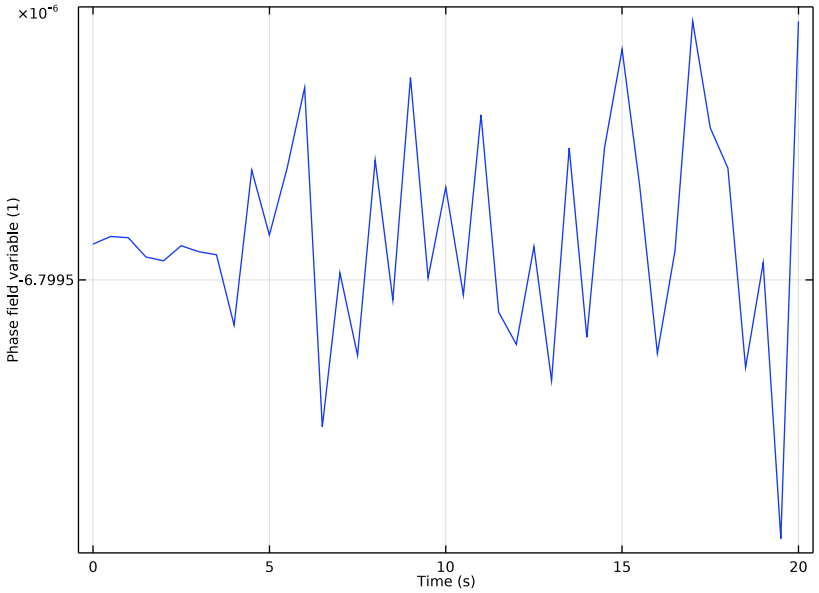

Figure 2: Plot of phase field variable integrated over the volume as a function of time. The total amount of mass in the system is perfectly conserved.

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, Canada, 2006.

Application Library path: `CFD_Module/Multiphase_Flow/phase_separation`

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 **Mathematics>Moving Interface>Phase Field (pf)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies>Time Dependent**.

6 Click **Done**.

GEOMETRY 1

Square 1 (sq1)

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

2 In the **Settings** window for **Square**, locate the **Size** section.

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

4 Click **Build All Objects**.

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

GLOBAL DEFINITIONS

Random 1 (rn1)

1 In the **Home** toolbar, click f(x) **Functions** and choose **Global>Random**.

2 In the **Settings** window for **Random**, type `phi_init` in the **Function name** text field.

3 Locate the **Parameters** section. In the **Number of arguments** text field, type `2`.

4 In the **Range** text field, type `0.1`.

PHASE FIELD (PF)

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Phase Field (pf)**.

2 In the **Settings** window for **Phase Field**, click to expand the **Discretization** section.

3 From the **Element order** list, choose **Quadratic**.

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 `0.08`.

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 From the **Phase field variable** list, choose **User defined**.

4 In the ϕ text field, type `phi_init(x[1/m],y[1/m])`.

MESH 1

Mapped 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Mapped**.

Size

1 In the **Settings** window for **Size**, locate the **Element Size** section.

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

3 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(0,0.5,20)`.

4 Click to expand the **Results While Solving** section. In the **Home** toolbar, click **Compute**.

RESULTS

Volume Fraction of Fluid 1 (pf)

1 In the **Settings** window for **2D Plot Group**, click to expand the **Title** section.

2 From the **Title type** list, choose **Custom**.

3 Find the **Type and data** subsection. Clear the **Type** check box.

4 Clear the **Description** check box.

5 Clear the **Unit** check box.

Volume Fraction of Fluid 1

1 In the **Model Builder** window, expand the **Volume Fraction of Fluid 1 (pf)** node, then click **Volume Fraction of Fluid 1**.

2 In the **Settings** window for **Surface**, click to expand the **Range** section.

3 Select the **Manual color range** check box.

4 In the **Minimum** text field, type `0.499`.

5 In the **Maximum** text field, type `0.501`.

6 Locate the **Coloring and Style** section. From the **Color table** list, choose **GrayScale**.

7 Right-click **Volume Fraction of Fluid 1** and choose **Show Legends**.

Volume Fraction of Fluid 1 (pf)

1 In the **Model Builder** window, click **Volume Fraction of Fluid 1 (pf)**.

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

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

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

Compare the resulting plot with that in the upper left panel of Figure 1.To create the remaining plots, plot the solution for the time values 1, 2, 4, 10, and 20 s .

Follow the steps below to reproduce the plot in Figure 2.

Surface Average 1

1 In the **Results** toolbar, click **More Derived Values** and choose **Average> Surface Average**.

2 Select Domain 1 only.

3 In the **Settings** window for **Surface Average**, click **Replace Expression** in the upper-right corner of the **Expressions** section. From the menu, choose **Component 1 (comp1)> Phase Field>phipf - Phase field variable**.

4 Click **Evaluate**.

TABLE

1 Go to the **Table** window.

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

It can be seen that the mass is conserved throughout the simulation.