COMSOL Implementation of Phase-Separation Model

Mark Fasano

Problem Statement

The model consists of two governing equations for the concentration profile of the oil ϕ, and the pressure p:

$$\phi_t + \nabla \cdot (\vec{u}_o \phi) = M \nabla \cdot \left(\phi \nabla \frac{\delta E}{\delta \phi} \right) \tag{1}$$

$$-\phi_t + \nabla \cdot (\vec{u}_w (1-\phi)) = -M \nabla \cdot \left(\phi \nabla \frac{\delta E}{\delta \phi} \right) \tag{2}$$

with corresponding flow described by

$$\vec{u}_o = -\tilde{k}_o \left[\nabla p + \rho \nabla \psi - \frac{\delta E}{\delta \phi} \nabla \phi \right] - k_o (1-\phi) \nabla \frac{\delta E}{\delta \phi} \tag{3}$$

$$\vec{u}_w = -\tilde{k}_w \left[\nabla p + \rho \nabla \psi - \frac{\delta E}{\delta \phi} \nabla \phi \right] + k_w \phi \nabla \frac{\delta E}{\delta \phi} \tag{4}$$

Here, k, k_o, and k_w are positive mobility coefficients with $\tilde{k}_i = k + k_i$, and M is a positive, diffusion mobility. The SAW effects are incorporated by creating a new effective pressure of the system, $\tilde{p} = p + \rho \psi$, where ρ is a matched density for the binary mixture (an assumption of the model) and ψ will take the form of the exponential below as per previous research *:

$$\psi = (1+\lambda^2) A^2 \omega^2 e^{-\alpha(x+\lambda z)} \tag{5}$$

Notice, α is an inverse attenutation length for the SAW wave in the x-direction, $(\lambda\alpha)^{-1}$ is the attenuation length in the z-direction, $\omega = 2\pi f$ is the angular frequency, and A is the maximum amplitude of the vertical displacements at the surface of the solid substrate due to the SAW. We consider the SAW acting on both components of the mixture with the only difference being captured in the coefficients $\tilde{k}_o, \tilde{k}_w$. Further, in accordance with Cahn-Hilliard theory, we use an approximate double-well potential for the homogeneous free engergy:

$$f(\phi) = \frac{\tilde{E}}{4} \phi^2 (1-\phi)^2 \tag{6}$$

See Appendix B for a detailed look at the parameter values investigated.

Non-Dimensionalization

We start by non-dimensionalizing equations 3-4 with the assumption that the length scale in both the x and z directions is the same. Hence, we scale:

$$(x,z) = \frac{1}{\alpha}(\hat{x}, \hat{z}), \quad (u_o, v_o, u_w, v_w) = \frac{1}{\alpha T}(\hat{u}_o, \hat{v}_o, \hat{u}_w, \hat{v}_w), \quad \tilde{p} = \Pi \hat{p}, \quad t = T\hat{t}, \quad f = \bar{E}\hat{f} \tag{7}$$

where $\Pi = \rho(1+\lambda^2)A^2\omega^2$, $\hat{\psi} = e^{-(x+\lambda z)}$ and T is to be determined. Considering 3, to simplify we choose $T = \frac{1}{\alpha^2 k_w \psi_o}$. With these scalings, and dropping hats henceforth for convenience, the dimensionless form of 3-4 is

$$\vec{u}_o = -(\kappa_0 + \kappa_1) \left[\nabla p - \left(\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right) \nabla \phi \right] - \kappa_0 (1-\phi) \nabla \left[\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right] \tag{8}$$

$$\vec{u}_w = -(1 + \kappa_1) \left[\nabla p - \left(\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right) \nabla \phi \right] + \phi \nabla \left[\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right] \tag{9}$$

where we have defined the following nondimensional parameters

$$\mathcal{E} = \frac{\bar{E}}{\Pi}, \quad \varepsilon^2 = \frac{\epsilon^2 \alpha^2}{\Pi}, \quad \kappa_0 = \frac{k_o}{k_w}, \quad \kappa_1 = \frac{k}{k_w}, \quad \mathcal{M} = \frac{M}{k_w} \tag{10}$$

*Shiokawa, Matsui, Ueda (1989)

Further, the dimensionless governing equations 1-2 are:

$$\phi_t + \nabla \cdot [\phi \vec{u}_o] = \nabla \cdot \left[\mathcal{M} \phi \nabla \left(\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right) \right] \tag{11}$$

$$-\phi_t + \nabla \cdot (\vec{u}_w (1-\phi)) = -\nabla \cdot \left(\mathcal{M} \phi \nabla \left(\mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \right) \right) \tag{12}$$

Now, we can define the dimensionless auxillary variables:

$$\mu = \mathcal{E} f'(\phi) - \varepsilon^2 \nabla^2 \phi \tag{13}$$

$$\vec{P} = \nabla p - \mu \nabla \phi \tag{14}$$

so that the flow may be written more concisely as:

$$\vec{u}_o = -(\kappa_0 + \kappa_1) \vec{P} - \kappa_0 (1-\phi) \nabla \mu \tag{15}$$

$$\vec{u}_w = -(1+\kappa_1) \vec{P} + \phi \nabla \mu \tag{16}$$

To model this in Comsol, we define our dependent variables as:

$$\vec{u} = (\phi, p, \mu, P_1, P_2)^T = (u_1, u_2, u_3, u_4, u_5)^T \tag{17}$$

with governing equations given by 11, 12, 13 and 14. Below, we rewrite these equations into Comsol's PDE Coefficients Form and list the non-zero coefficients:

For $i = 1$:

$$\frac{\partial u_1}{\partial t} + \frac{\partial}{\partial x_1} \left[-((\kappa_0 + \kappa_1) u_1) u_4 - (\kappa_0 u_1 (1-u_1) + \mathcal{M} u_1) \frac{\partial u_3}{\partial x_1} \right] + \frac{\partial}{\partial x_2} \left[-((\kappa_0 + \kappa_1) u_1) u_5 - (\kappa_0 u_1 (1-u_1) + \mathcal{M} u_1) \frac{\partial u_3}{\partial x_2} \right] = 0 \tag{18}$$

with non-zero coefficients

$$\boxed{d_{11} = 1, \quad \alpha_{141} = \alpha_{152} = (\kappa_0 + \kappa_1) u_1, \quad c_{1311} = c_{1322} = \kappa_0 u_1 (1-u_1) + \mathcal{M} u_1} \tag{19}$$

For $i = 2$:

$$-\frac{\partial u_1}{\partial t} + \frac{\partial}{\partial x_1} \left[-(1+\kappa_1)(1-u_1) u_4 + (u_1(1-u_1) + \mathcal{M} u_1) \frac{\partial u_3}{\partial x_1} \right] + \frac{\partial}{\partial x_2} \left[-(1+\kappa_1)(1-u_1) u_5 + (u_1(1-u_1) + \mathcal{M} u_1) \frac{\partial u_3}{\partial x_2} \right] = 0 \tag{20}$$

with non-zero coefficients

$$\boxed{d_{21} = -1, \quad \alpha_{241} = \alpha_{252} = (1+\kappa_1)(1-u_1), \quad c_{2311} = c_{2322} = -u_1(1-u_1) - \mathcal{M} u_1} \tag{21}$$

For $i = 3$:

$$\varepsilon^2 \left(\frac{\partial^2 u_1}{\partial x_1^2} + \frac{\partial^2 u_1}{\partial x_2^2} \right) + u_3 = \mathcal{E} f'(\phi) \tag{22}$$

with non-zero coefficients

$$\boxed{c_{3111} = c_{3122} = -\varepsilon^2, \quad a_{33} = 1, \quad f_3 = \mathcal{E} f'(\phi)} \tag{23}$$

For $i = 4$:

$$-\frac{\partial u_2}{\partial x_1} + u_3 \frac{\partial u_1}{\partial x_1} + u_4 = 0 \tag{24}$$

with non-zero coefficients

$$\boxed{\beta_{421} = -1, \quad \beta_{411} = u_3, \quad a_{44} = 1} \tag{25}$$

For $i = 5$:

$$-\frac{\partial u_2}{\partial x_2} + u_3 \frac{\partial u_1}{\partial x_2} + u_5 = 0 \tag{26}$$

with non-zero coefficients

$$\boxed{\beta_{522} = -1, \quad \beta_{512} = u_3, \quad a_{55} = 1} \tag{27}$$

Taking a detailed look at the Comsol "No-Flux" condition given by:

$$\mathbf{n} \cdot (c\nabla\vec{u} + \alpha\vec{u} - \gamma) = 0 \implies n_l \left(c_{ijkl} \frac{\partial u_j}{\partial x_k} + \alpha_{ijl} u_j - \gamma_{il} \right) = 0 \tag{28}$$

we can see that for the model described above, the boundary conditions this is enforcing at $x = 0, 1$ are

$$\begin{bmatrix} c_{1311} \frac{\partial \mu}{\partial x} + \alpha_{141} P_1 \\ c_{2311} \frac{\partial \mu}{\partial x} + \alpha_{241} P_1 \\ c_{3111} \frac{\partial \phi}{\partial x} \\ 0 \\ 0 \end{bmatrix} = \vec{0}$$

and at $z = 0, 1$ the boundary conditions are

$$\begin{bmatrix} c_{1322} \frac{\partial \mu}{\partial z} + \alpha_{152} P_2 \\ c_{2322} \frac{\partial \mu}{\partial z} + \alpha_{252} P_2 \\ c_{3122} \frac{\partial \phi}{\partial z} \\ 0 \\ 0 \end{bmatrix} = \vec{0}$$

In terms of ϕ and p, these boundary conditions amount to the following at $x = 0, 1$:

$$\begin{bmatrix} [\kappa_0 \phi(1-\phi) + \mathcal{M}\phi] \left(\mathcal{E} f''(\phi)\phi_x - \varepsilon^2(\phi_{xxx} + \phi_{zzx}) \right) + [(\kappa_0 + \kappa_1)\phi] \left(p_x - \left(\mathcal{E} f'(\phi) - \varepsilon^2(\phi_{xx} + \phi_{zz}) \right) \phi_x \right) \\ - [\phi(1-\phi) + \mathcal{M}\phi] \left(\mathcal{E} f''(\phi)\phi_x - \varepsilon^2(\phi_{xxx} + \phi_{zzx}) \right) + [(1 + \kappa_1)(1-\phi)] \left(p_x - \left(\mathcal{E} f'(\phi) - \varepsilon^2(\phi_{xx} + \phi_{zz}) \right) \phi_x \right) \\ -\varepsilon^2 \phi_x \\ 0 \\ 0 \end{bmatrix} = \vec{0}$$

and at $z = 0, 1$ the boundary conditions are

$$\begin{bmatrix} [\kappa_0 \phi(1-\phi) + \mathcal{M}\phi] \left(\mathcal{E} f''(\phi)\phi_z - \varepsilon^2(\phi_{xxz} + \phi_{zzz}) \right) + [(\kappa_0 + \kappa_1)\phi] \left(p_z - \left(\mathcal{E} f'(\phi) - \varepsilon^2(\phi_{xx} + \phi_{zz}) \right) \phi_z \right) \\ - [\phi(1-\phi) + \mathcal{M}\phi] \left(\mathcal{E} f''(\phi)\phi_z - \varepsilon^2(\phi_{xxz} + \phi_{zzz}) \right) + [(1 + \kappa_1)(1-\phi)] \left(p_z - \left(\mathcal{E} f'(\phi) - \varepsilon^2(\phi_{xx} + \phi_{zz}) \right) \phi_z \right) \\ -\varepsilon^2 \phi_z \\ 0 \\ 0 \end{bmatrix} = \vec{0}$$

Appendix A

COMSOL Multiphysics formulation of PDE Coefficients Form solves, by finite elements, a vectorial equation for the unknown vector $\vec{u} = (u_1, u_2, ..., u_N)^T$ which reads as:

$$\boldsymbol{e}\frac{\partial^2 \vec{u}}{\partial t^2} + \boldsymbol{d}\frac{\partial \vec{u}}{\partial t} + \nabla \cdot (-\boldsymbol{c}\nabla\vec{u} - \alpha\vec{u} + \gamma) + \beta\nabla\vec{u} + \boldsymbol{a}\vec{u} = \vec{f} \tag{29}$$

where the coefficients of the N scalar equations are in the matrices $\boldsymbol{e}, \boldsymbol{d}, \gamma, \boldsymbol{a}$ (of dimensions $N \times N$), α, β (of dimensions $N \times N \times n$), $\boldsymbol{c}$ (of dimensions $N \times N \times n \times n$) and the vector $\vec{f}$ (of dimension N), where n is the spatial dimension of the problem ($n = 1, 2, 3$). In index notation, this expression reads as

$$e_{ij}\frac{\partial^2 u_j}{\partial t^2} + d_{ij}\frac{\partial u_j}{\partial t} + \frac{\partial}{\partial x_l}\left(-c_{ijkl}\frac{\partial u_j}{\partial x_k} - \alpha_{ijl}u_j + \gamma_{il}\right) + \beta_{ijl}\frac{\partial u_j}{\partial x_l} + a_{ij}u_j = f_i \tag{30}$$

where $i, j = 1, ..., N$ and $k, l = 1, ..., n$.

Appendix B

In this section, we provide a complete list of parameters and variables in the problem with their dimensions, numerical values, and a brief description:

Parameter	Value	Fundamental Unit	Description
k		$\frac{L^3T}{M}$	Mobility coefficient for mass-averaged velocity
k_o		$\frac{L^3T}{M}$	Mobility coefficient for oil
k_w		$\frac{L^3T}{M}$	Mobility coefficient for water
M		$\frac{L^3T}{M}$	Diffusion mobility coefficient
$\tilde{E}$		$\frac{M}{LT^2}$	Energy coefficient from CH Theory
ϵ^2		$\frac{ML}{T^2}$	Width of the diffuse interface from CH Theory
ρ		$\frac{M}{L^3}$	Matched density of mixture
A		L	Maximum amplitude of vertical displacements at surface due to SAW
α		$\frac{1}{L}$	Inverse attenuation length for SAW in x
ω		$\frac{1}{T}$	Angular frequency of SAW
λ		1	$(\lambda\alpha)^{-1}$ is attenuation length for SAW in z