

# Numerical simulation of interfacial mass transfer using the immersed interface method

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**Abstract.** The immersed interface method (IIM) is a Cartesian grid method with second order accuracy and has been applied to many immersed boundary problems. The IIM has seen further improvement by many subsequent researchers and has proven to be fairly robust and accurate for problems involving immersed impermeable deformable boundaries. However, efforts to extend this numerical technique for permeable boundary problems are still rather lacking. In the present work, mass transfer across an interface between two immiscible fluids is simulated using the IIM. The same viscosities for the two phases and the instantaneous thermodynamic equilibrium at the interface are assumed. The numerical results suggest that the method is deemed capable of simulating the aforementioned mass transfer mechanism.

**Key Words:** Immersed interface method, Simulation, Mass transfer, Stokes flows

## 1. Introduction

The immersed interface method (IIM) was developed by LeVeque and Li (1994) with second order accuracy. Layton (2006) and Jayathilake *et al.* (2010a) reported some extensions for the IIM to simulate a permeable capsule immersed in a binary solution under the Stokes flow condition. Recently, this approach was further extended for problems involved in capsule-substrate adhesion in the presence of osmosis (Jayathilake *et al.* 2010b).

In the present work, the IIM model reported in Jayathilake *et al.* (2010a,b) is extended to simulate two-phase fluid flow in two dimension, taking into account mass transport of a dissolved dilute solute and its interfacial mass transfer. The Stokes flow problem is solved by decoupling the Stokes equations into three Poisson equations each for pressure and two velocity components (LeVeque and Li 1997). The solute transfer is described by the species transport equation, and the thermodynamic equilibrium is assumed at the interface. The discontinuity of the solute concentration field is incorporated into the finite difference scheme of the

species transport equation by calculating the approximate concentration jump conditions at the interface. The numerical simulations are performed for both the fixed and moving interface problems.

## 2. Model formulation and numerical method

The calculation procedure used in Jayathilake *et al.* (2010a) can be extended easily to simulate a rising droplet with mass transfer between the droplet (i.e., dispersed phase) and the surrounding fluid (i.e., continuous phase) (see Figure 1). The viscosities for the two phases are considered as the same. The Stokes flow is assumed and the governing equations are as below:

$$p_x(x, y, t) = \mu(u_{xx}(x, y, t) + u_{yy}(x, y, t)) + F_1(x, y, t), \quad (1)$$

$$p_y(x, y, t) = \mu(v_{xx}(x, y, t) + v_{yy}(x, y, t)) + F_2(x, y, t) - g\rho, \quad (2)$$

$$u_x(x, y, t) + v_y(x, y, t) = 0, \quad (3)$$

$$\begin{aligned} c_t(x, y, t) + u(x, y, t).c_x(x, y, t) + v(x, y, t).c_y(x, y, t) \\ = D(c_{xx}(x, y, t) + c_{yy}(x, y, t)). \end{aligned} \quad (4)$$

Here,  $p$  and  $(u, v)$  are the fluid pressure and fluid velocity, respectively.  $\mu$  is the dynamic viscosity and it is the same for both phases.  $c$  is the solute concentration and  $D$  is the solute diffusivity.

The interfacial forces arise due to the surface tension and hence the force strength is computed as

$$\vec{f} = (ST) \frac{\partial^2 \vec{X}(s, t)}{\partial s^2}, \quad (5)$$

where,  $ST$  is the coefficient of surface tension.

For a permeable membrane, the interfacial mass transfer is governed by the Kedem-Katchalsky equations. Similarly, for the rising droplet, Henry's law is employed to compute interfacial mass transfer. Therefore,  $c_2/c_1 = H$ , where  $H$  is the Henry's coefficient. The second interfacial condition is that the solute mass continuity across the interface given by  $D_1 \frac{\partial c_1}{\partial n} = D_2 \frac{\partial c_2}{\partial n}$ . Here,  $c_1$  and  $c_2$  are the solute concentrations in the dispersed and continuous phases, respectively, and  $D_1$  and  $D_2$  are respective diffusion coefficients.  $n$  is the outward normal vector to the interface.

The pressure and velocity are assumed periodic in the  $x$  direction. However, the periodic boundary condition for  $p$  in the  $y$  direction is not deemed reasonable due to the hydrostatic pressure gradient in the  $y$  direction. Therefore, the equations

of motion are reformulated as reported in LeVeque and Li (1997) by defining a new variable  $\hat{p}$  as  $p = g\rho_0(b_2 - b_1 - y) + \hat{p}$ . Indeed,  $\hat{p}$  is the pressure fluctuation from the hydrostatic pressure. Then, Eqs. (1) and (2) are reformulated as

$$\hat{p}_x(x, y, t) = \mu(u_{xx}(x, y, t) + u_{yy}(x, y, t)) + F_1(x, y, t), \tag{6}$$

$$\hat{p}_y(x, y, t) = \mu(v_{xx}(x, y, t) + v_{yy}(x, y, t)) + F_2(x, y, t) - g(\rho - \rho_0), \tag{7}$$

where,  $\rho_0 = \frac{1}{(a_2 - a_1)(b_2 - b_1)} \iint_{\Omega} \rho(x, y) dx dy$  is the average density of the whole fluid domain.

The jump conditions for pressure and velocity are given by  $[\hat{p}] = f_n$ ,  $[\hat{p}_n] = g[\rho] \sin \theta$ ,  $[u] = [v] = 0$ ,  $[u_n] = [v_n] = 0$ , where  $\theta$  is the angle between the  $n$  and the  $x$  directions. Following LeVeque and Li (1997), the equations of motion Eqs. (1), (2), and (3) are solved by decoupling them into three Poisson equations as  $\nabla^2 \hat{p} = \nabla \vec{F} - g\rho_y$ ,  $\nabla^2 u = (\hat{p}_x - F_1)/\mu$ ,  $\nabla^2 v = (\hat{p}_y - F_2 + g(\rho - \rho_0))/\mu$  each for  $p$ ,  $u$  and  $v$ , respectively.

The transport equation Eq. (4) is solved separately in two phases (i.e., dispersed and continuous phases) since the solute diffusivity ( $D$ ) may be different for two phases ( $D_1, D_2$ ). The discontinuity of the concentration field is avoided by defining a new variable  $\hat{c}$  as  $\hat{c} = c_1 H$  for the dispersed phase and  $\hat{c} = c_2$  for the continuous phase. Then, the modified transport equation is

$$\begin{aligned} \hat{c}_t(x, y, t) + u(x, y, t) \cdot \hat{c}_x(x, y, t) + v(x, y, t) \cdot \hat{c}_y(x, y, t) \\ = D_{1,2}(\hat{c}_{xx}(x, y, t) + \hat{c}_{yy}(x, y, t)). \end{aligned} \tag{8}$$

Then, the new interfacial conditions are  $[\hat{c}] = 0$  and  $D_1 \frac{\partial \hat{c}_1}{\partial n} = H D_2 \frac{\partial \hat{c}_2}{\partial n}$ . It should be noted that the continuous concentration field  $\hat{c}$  is not smooth across the interface. Therefore, correction terms for the transport equation are still needed. Thus, jump of normal derivative  $[\hat{c}_n]$  is computed numerically to calculate for the correction terms. By discretizing the interfacial condition  $D_1 \frac{\partial \hat{c}_1}{\partial n} = H D_2 \frac{\partial \hat{c}_2}{\partial n}$  along the normal line at the  $k^{\text{th}}$  control point on the interface, the concentration at the immediate sides of the interface is obtained as

$$c_k^{\pm, m+1} = \frac{\{H D_2 (4\hat{c}_{k,3}^{m+1} - \hat{c}_{k,4}^{m+1}) + D_1 (4\hat{c}_{k,1}^{m+1} - \hat{c}_{k,2}^{m+1})\}}{3(H D_2 + D_1)}. \tag{9}$$

Then, the concentration jump conditions are  $[\hat{c}]^{m+1} = 0$ ,  $[\hat{c}_{n,k}]^{m+1} = \hat{c}_{n,k}^{+, m+1} - \hat{c}_{n,k}^{-, m+1}$ . Next, Eq. (8) is solved by explicit discretization to compute for  $c$ .

### 3. Results and discussion

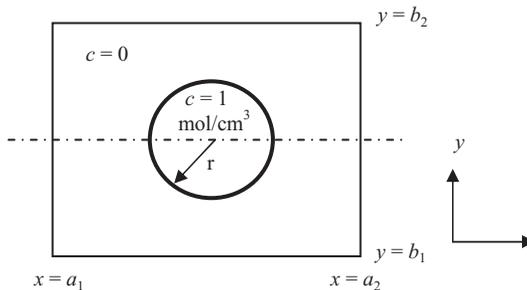
In this preliminary work, the results are presented for the validation of the present numerical method as opposed to detailed numerical investigations on mass transfer between two phases. First the numerical method is validated for mass transfer between two phases having a fixed interface between them. Second, the validation is given for a rising droplet with mass transfer across the interface.

#### 3.1 Fixed interface problem

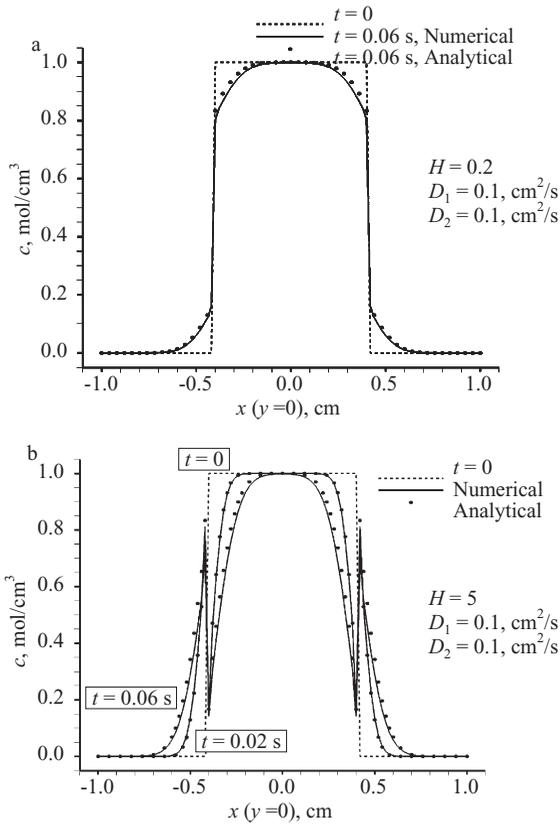
The droplet having a radius of 0.4 cm is immersed in a square computational domain of 2 x 2 cm as shown in Figure 1. The solute concentrations in the droplet and surrounding field are 1 and 0 mol/cm<sup>3</sup>, respectively. Figures 2 and 3 show the concentration fields on  $y=0$  plane for different diffusivities and Henry's numbers. The numerical results are compared with an analytical solution given in Onea (2007). It is seen that the transient variation of solute concentration field have excellent agreement with the analytical solutions at the beginning of mass transfer.

Theoretically, it is known that the non-dimensional mass transfer coefficient, Sherwood number  $Sh$ , for a fixed circular interface problem is 2.0 at the steady state. An initially unsteady concentration field in a fixed circular interface problem is simulated using the present method and the transient variation of  $Sh$  is shown in Figure 4.  $Sh$  is defined as the ratio between the average mass flux across the interface and the average of the concentration difference between the interface and the far field (Deshpande and Zimmerman 2006). The numerical value of  $Sh$  reaches the steady state value of 2 consistent with the theoretical value.

Furthermore, the present method is used to simulate oxygen transport between an air bubble and surrounding water. It seems that the method could simulate the aforementioned problem successfully (results not shown).



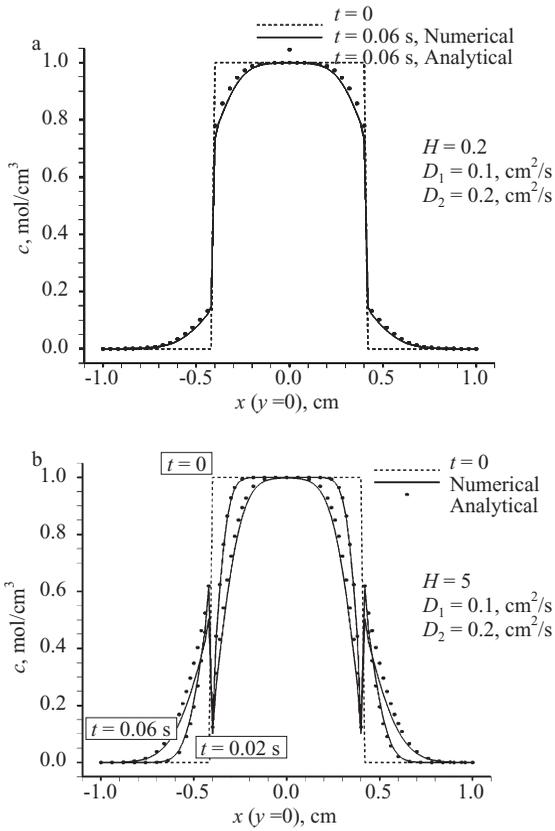
**Figure 1** Schematic diagram for the fixed interface problem.



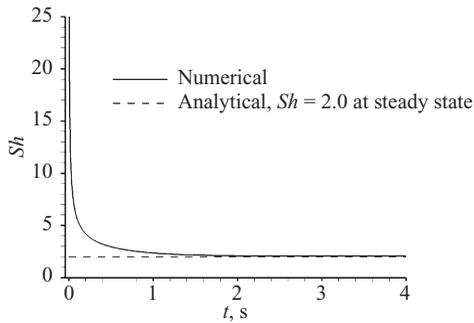
**Figure 2** Comparison for the fixed interface problem at the same diffusivities. (a)  $H=0.2$  (b)  $H=5$ .

### 3.2 Moving interface problem

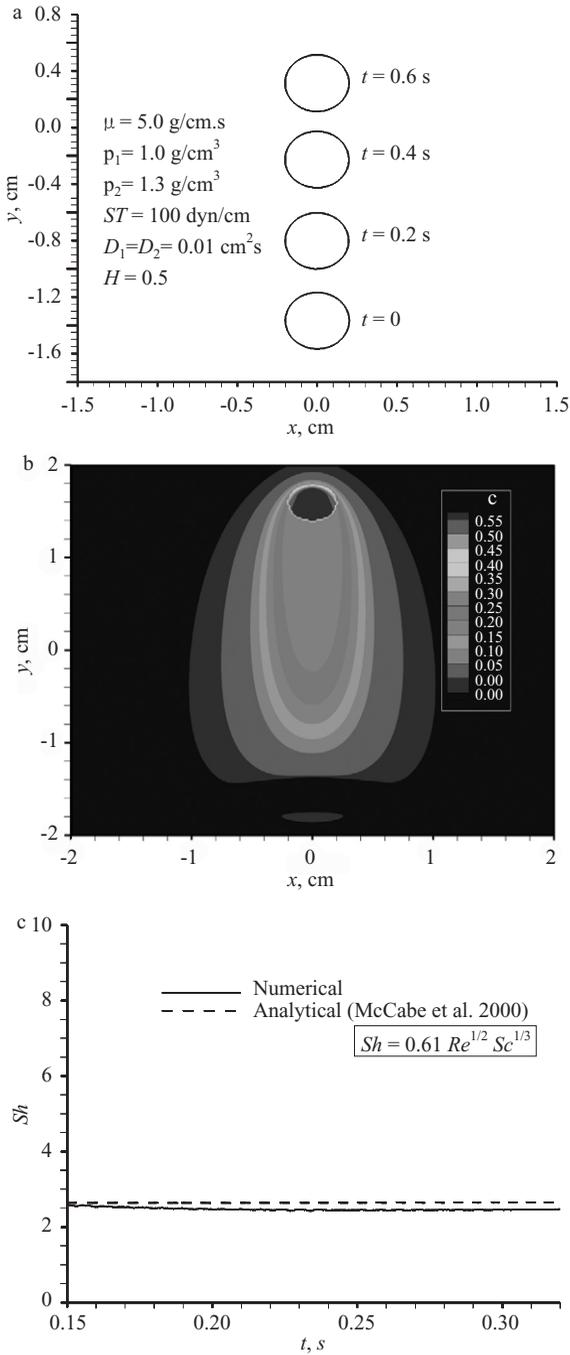
Next, a rising droplet is simulated and the transient variation of  $Sh$  is compared with an empirical solution reported in McCabe *et al.* (2000). A droplet having a radius of 0.2 cm rises in a square fluid domain of 4 x 4 cm. The initial solute concentration of droplet and the surrounding field are 1 and 0 mol/cm<sup>3</sup>, respectively. The Henry’s number is 0.5. Figure 5 shows the rising droplet, the concentration field when the droplet reaches  $y=1.8$  cm, and the transient variation of  $Sh$ . The droplet is almost undeformed for the selected properties and it is consistent with results given in Clift *et al.* (1978). When the capsule rises, some solute diffuses into the surrounding field is seen in Figure 5(b). As can be seen in Figure 5(c), the numerical and empirical values for  $Sh$  are close in magnitude hence further validating the numerical method.



**Figure 3** Comparison for the fixed interface problem at different diffusivities. (a)  $H=0.2$  (b)  $H=5$ .



**Figure 4** Comparison for the Sherwood number,  $Sh$ .



**Figure 5** A rising droplet with mass transfer across the interface. (a) rising droplet (b) concentration field (c) comparison for  $Sh$ .

## 4. Conclusions

Mass transfer across an interface between two immiscible fluids is simulated using the immersed interface method (IIM). The present method is employed to both fixed and moving interface problems to validate the present numerical method.

All the validation tests suggest that the present numerical procedure based on the IIM is deemed reasonable for simulating mass transfer between two phases including a rising droplet and a surrounding field under the Stokes flow assumption. The present method would be improved for different viscosities for the two phases so that it can be used to simulate a rising bubble too.

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