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Supplement to
"Lubrication pressure model in a non-negligible gap for fluid permeation through a membrane with finite permeability"

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In this supplementary material, the numerical method for solving permeation flow through membrane is summarised based on our consistent direct discretisation approach [1, 2, 3] for the discrete-forcing (DF) immersed boundary (IB) method.

1 Numerical method

Immersed boundary methods are widely employed for solving fluid-structure interaction problems on a fixed mesh that does not conform to the object surface. Among these methods, the DF-IB approach offers a sharp interface treatment by incorporating the boundary conditions of the interfacial velocity into the discretised governing equations. For the DF-IB approach, one of the present authors developed a concept of "consistent discretisation" [4] of the pressure equation with that of the Navier-Stokes (N-S) equation (or "consistent coupling" of the incompressible velocity and pressure fields), which considers the distance from the interface to the adjacent-cell centre for discretising the pressure Poisson equation to strictly satisfy the mass conservation at the boundary cells [4]. Sato et al. [1] and Takeuchi et al. [2] further developed a method that directly discretises the N-S equation even at the grid points adjacent to the interface, while simultaneously ensuring consistency between the incompressible velocity and pressure fields. By using their "consistent direct discretisation" for the DF-IB approach, the non-slip condition on the interface was strictly imposed in a discrete sense while satisfying the mass and momentum conservations, which allows the sharp distribution of the velocity and pressure at the interface to be captured. This idea is in contrast with the strategy of early DF-IB approaches (including Ref. [4]), which complete the time integration of the velocity at the boundary cell by simply assigning an interpolated value (without solving the equation of motion in the vicinity of the interface).

Takeuchi et al. [3] coupled the above system with the permeate condition at the interface and derived a new pressure Poisson equation for a system with a permeable membrane for solvent. Based on Ref. [5], the consistent direct discretisation with a permeable interface is briefly summarised in the following.

1.1 Governing equations

The governing equations of a fluid are the equation of continuity and the Navier-Stokes equation, and the non-dimensional forms according to the reference velocity U and the reference length H are as follows:

$$\nabla \cdot \boldsymbol{u} = 0 \,, \tag{1}$$

$$\frac{\partial \boldsymbol{u}}{\partial t} + \boldsymbol{u} \cdot \nabla \boldsymbol{u} = -\nabla p + \frac{\nabla^2 \boldsymbol{u}}{\mathrm{Re}} \,. \tag{2}$$

Here, $\boldsymbol{u}$ is the velocity, t the time, p the pressure non-denationalised by ρU^2, and Re is the Reynolds number.

The volumetric flux of the pure fluid (i.e. fluid without any solute) across the membrane is expressed in a non-dimensional form as follows:

$$\boldsymbol{J} = \mathrm{Re}\mathcal{L} \, [\![p]\!] \, \boldsymbol{n} \,, \tag{3}$$

where $\mathcal{L}$ is the non-dimensional permeable coefficient defined as $L_{\mathrm{p}}\mu/H$ with L_{p} and μ being the dimensional permeability and viscous coefficient, respectively; $[\![p]\!]$ is the discontinuity of the pressure across the membrane, and $\boldsymbol{n}$ is the unit normal vector.

1.2 Spatial discretisation

The governing equations are discretised using a finite difference method. The flow variables are defined on the collocated arrangement, and the spatial discretisation is given by a second-order central finite difference. The convective and viscous terms are time-updated using the 4th-order Runge-Kutta method. A fractional-step method is employed to couple the velocity and pressure fields.

Figure S1 shows the schematic of a membrane in an incompressible fluid in two dimensions. Hereafter, the computational cells partitioned by the object boundary (as represented by the triangular symbol in the figure) are referred to as "boundary cells". For the boundary cell (i, j) shown in Fig. S1, the discretisations incorporating the boundary conditions are explained in two dimensions.

In the following, $\overline{(\cdot)}$ represents an interpolation operator of the second-order accuracy, and δ_{x_k} is an operator of second-order central finite difference in the x_k direction. The velocities at the cell face are denoted by $U_k (k = 1, 2)$ or (U, V), and the fractional-step velocities (by excluding the pressure gradient) at the cell centre and cell face are represented by u^{**} and U_k^{**}, respectively. The subscripts "$b \mp 0$" represent

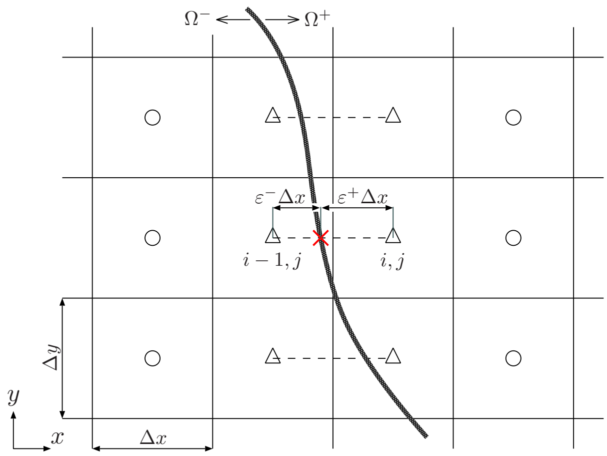


Figure S1: Schematic of membrane (immersed object) on a fixed Cartesian mesh system. The boundary cells are labelled by a triangular symbol, and the other fluid cells are represented by a circular symbol. The grid lines of the boundary cells $(i-1,j)$-(i,j) are separated by a permeable membrane. The intersecting point of the membrane with the grid line connecting the centres of the boundary cells is represented by "$\times$" symbol.

the limiting values on the left- and right-hand sides of the interface ($\Omega^{\mp}$ in Fig. S1), and $\phi_k (k = 3, 4, 5)$ are the interpolation/extrapolation functions applied to the boundary cells (given later).

In the following, the discretisations in the boundary cells are presented based on the configuration in Fig. S1 to show the treatments considering the distance between the surface and the cell centre.

The discretisations for the convective and viscous terms are as follows:

- Convective term at $(i-1,j)$

$$\left[\frac{\partial (U_k u)}{\partial x_k}\right]_{i-1,j} = \frac{1}{\Delta x}\left\{U_{i-\frac{1}{2},j}\left[\phi_3^-(u)\right]_{i-\frac{1}{2},j} - U_{i-\frac{3}{2},j}\left(\overline{u}^x\right)_{i-\frac{3}{2},j}\right\} + \frac{1}{\Delta y}\left\{V_{i-1,j+\frac{1}{2}}\left(\overline{u}^y\right)_{i-1,j+\frac{1}{2}} - V_{i-1,j-\frac{1}{2}}\left(\overline{u}^y\right)_{i-1,j-\frac{1}{2}}\right\} \quad (4)$$

- Convective term at (i,j)

$$\left[\frac{\partial (U_k u)}{\partial x_k}\right]_{i,j} = \frac{1}{\Delta x}\left\{U_{i+\frac{1}{2},j}\left(\overline{u}^x\right)_{i+\frac{1}{2},j} - U_{i-\frac{1}{2},j}\left[\phi_3^+(u)\right]_{i-\frac{1}{2},j}\right\} + \frac{1}{\Delta y}\left\{V_{i,j+\frac{1}{2}}\left(\overline{u}^y\right)_{i,j+\frac{1}{2}} - V_{i,j-\frac{1}{2}}\left(\overline{u}^y\right)_{i,j-\frac{1}{2}}\right\} \quad (5)$$

- Viscous term at $(i-1,j)$

$$\frac{1}{\mathrm{Re}}\left[\frac{\partial^2 u}{\partial {x_j}^2}\right]_{i-1,j} = \frac{1}{\mathrm{Re}}\left[\frac{1}{0.5\left(\varepsilon^- + 1\right)\Delta x}\left\{\left(\frac{u_{b-0} - u_{i-1,j}}{\varepsilon^-\Delta x}\right) - \left(\delta_x u\right)_{i-\frac{3}{2},j}\right\} + \left(\delta_y\delta_y u\right)_{i-1,j}\right] \quad (6)$$

- Viscous term at (i,j)

$$\frac{1}{\mathrm{Re}}\left[\frac{\partial^2 u}{\partial {x_j}^2}\right]_{i,j} = \frac{1}{\mathrm{Re}}\left[\frac{1}{0.5\left(\varepsilon^+ + 1\right)\Delta x}\left\{\left(\delta_x u\right)_{i+\frac{1}{2},j} - \left(\frac{u_{i,j} - u_{b+0}}{\varepsilon^+\Delta x}\right)\right\} + \left(\delta_y\delta_y u\right)_{i,j}\right] \quad (7)$$

where the interpolation functions are

$$\left[\phi_3^-\left(u\right)\right]_{i-\frac{1}{2},j} = \frac{\left(\varepsilon^- - 0.5\right)u_{i-1,j} + 0.5u_{b-0}}{\varepsilon^-}\,, \tag{8}$$

$$\left[\phi_3^+\left(u\right)\right]_{i-\frac{1}{2},j} = \frac{\left(\varepsilon^+ - 0.5\right)u_{i,j} + 0.5u_{b+0}}{\varepsilon^+}\,, \tag{9}$$

and $\varepsilon^\mp$ are as shown in Fig. S1. For a moving boundary problem, the fluid velocity on the membrane $u_{b\mp0}$ must be specified to coincide with the sum of the translating velocity of membrane u_m and permeate flux component $\mathrm{Re}\mathcal{L}n_x\,[\![p]\!]$. As a general procedure in our study, the two neighbouring Lagrangian markers (consisting of the membrane) closest to the "$\times$" points in Fig. S1 are identified, and the membrane velocity u_m is determined by a linear interpolation of the marker velocities. Note that while the primary variables defined on the (collocated) cell centres are solved by the direct discretisation, the secondary variables (such as cell-face velocities and gradients) are obtained by interpolation and extrapolation.

The pressure fields associated with the permeate flux should satisfy the following equations on the respective sides of the membrane [3]:

- Permeated pressure equation in the boundary cell $(i-1,j)$

$$-\frac{\Delta t}{\left(\varepsilon^- + 0.5\right)\Delta x}\left\{\left(\delta_x p^{n+1}\right)_{i-\frac{3}{2},j} + \frac{\mathrm{Re}\mathcal{L}n_x^{n+1}\,[\![p]\!]^{n+1}}{\Delta t}\right\} + \Delta t\left(\delta_y\delta_y p^{n+1}\right)_{i-1,j} = \frac{u_m^{n+1} - U^{**}_{i-\frac{3}{2},j}}{\left(\varepsilon^- + 0.5\right)\Delta x} + \left(\delta_y V^{**}\right)_{i-1,j} \tag{10}$$

- Permeated pressure equation in the boundary cell (i,j)

$$\frac{\Delta t}{\left(\varepsilon^+ + 0.5\right)\Delta x}\left\{\left(\delta_x p^{n+1}\right)_{i+\frac{1}{2},j} + \frac{\mathrm{Re}\mathcal{L}n_x^{n+1}\,[\![p]\!]^{n+1}}{\Delta t}\right\} + \Delta t\left(\delta_y\delta_y p^{n+1}\right)_{i,j} = \frac{U^{**}_{i+\frac{1}{2},j} - u_m^{n+1}}{\left(\varepsilon^+ + 0.5\right)\Delta x} + \left(\delta_y V^{**}\right)_{i,j}\,, \tag{11}$$

To close the discretised equations above, $[\![p]\!]$ must be specified. In the implementation, the pressure jump is expressed with the difference between the two pressures separately extrapolated from the regions away from the interface on both sides of the membrane.

Finally, the time-update of the incompressible velocity is completed as follows:

- Velocity correction procedure at $(i-1,j)$

$$u_{i-1,j}^{n+1} = u_{i-1,j}^{**} - \Delta t \left[\phi_4^- \left(\frac{\delta p^{n+1}}{\delta x}\right)\right]_{i-1,j}, \tag{12}$$

$$U_{i-\frac{1}{2},j}^{n+1} = U_{i-\frac{1}{2},j}^{**} - \Delta t \left[\phi_5^- \left(\frac{\delta p^{n+1}}{\delta x}\right)\right]_{i-\frac{1}{2},j} \tag{13}$$

- Velocity correction procedure at (i,j)

$$u_{i,j}^{n+1} = u_{i,j}^{**} - \Delta t \left[\phi_4^+ \left(\frac{\delta p^{n+1}}{\delta x}\right)\right]_{i,j}, \tag{14}$$

$$U_{i-\frac{1}{2},j}^{n+1} = U_{i-\frac{1}{2},j}^{**} - \Delta t \left[\phi_5^+ \left(\frac{\delta p^{n+1}}{\delta x}\right)\right]_{i-\frac{1}{2},j} \tag{15}$$

where the interpolation functions are given as follows:

$$\left[\phi_4^- \left(\frac{\delta p}{\delta x}\right)\right]_{i-1,j} = \frac{1}{\varepsilon^- + 0.5}\left\{\varepsilon^- \left(\delta_x p\right)_{i-\frac{3}{2},j} + 0.5\left(\frac{\delta p}{\delta x}\right)_{b-0}\right\}, \tag{16}$$

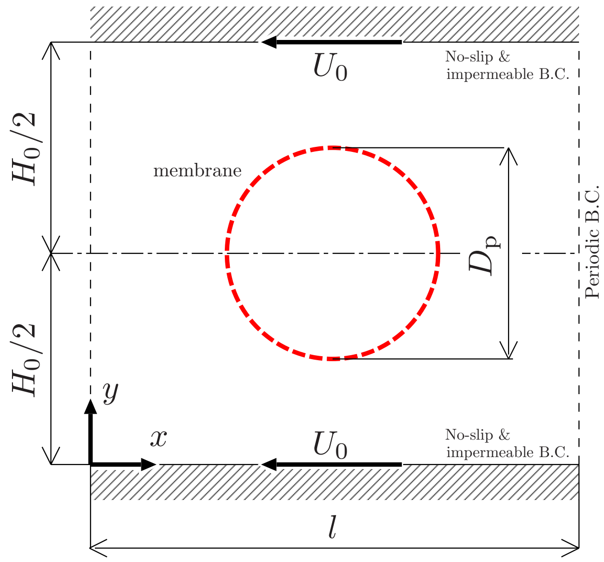
$$\left[\phi_5^- \left(\frac{\delta p}{\delta x}\right)\right]_{i-\frac{1}{2},j} = \frac{\varepsilon^- - 0.5}{\varepsilon^- + 0.5}\left(\delta_x p\right)_{i-\frac{3}{2},j}, \tag{17}$$

$$\left[\phi_4^+ \left(\frac{\delta p}{\delta x}\right)\right]_{i,j} = \frac{1}{\varepsilon^+ + 0.5}\left\{\varepsilon^+ \left(\delta_x p\right)_{i+\frac{1}{2},j} + 0.5\left(\frac{\delta p}{\delta x}\right)_{b+0}\right\}, \tag{18}$$

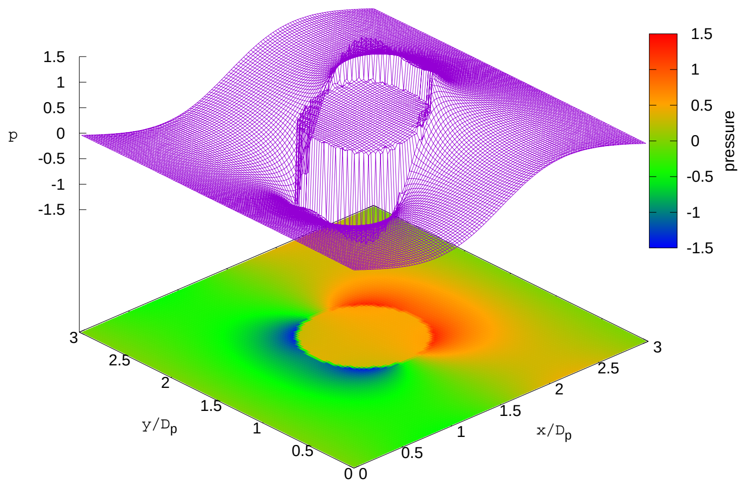
$$\left[\phi_5^+ \left(\frac{\delta p}{\delta x}\right)\right]_{i-\frac{1}{2},j} = \frac{\varepsilon^+ - 0.5}{\varepsilon^+ + 0.5}\left(\delta_x p\right)_{i+\frac{1}{2},j}. \tag{19}$$

As described above, by considering the distance to the object surface for discretising the equations, the momentum conservation is satisfied in a discrete sense, even in the boundary cell. This differs from the early DF-IB approaches that assigned the velocity near the interface by performing interpolation to satisfy the no-slip condition at the interface. Therefore, the above discretisation procedure claims "direct discretisation," even in the immediate vicinity of the interface. Furthermore, the correction procedure (Eqs. (12)∼ (15), using the pressure at the next time level obtained by solving the pressure Poisson equations (10) and (11)) determines the velocity in the boundary cell to satisfy the permeable condition at the interface; therefore, the mass is simultaneously conserved in a discrete sense. This procedure guarantees the consistency between the incompressible velocity and pressure fields.

The validity of the numerical method was assessed by comparing the numerical result of permeate flow rate with the analytical models for different permeabilities over six orders of magnitude (i.e. $\mathcal{L} = 10^{-3}$ to 10^3) [3]. The method was found to reproduce a sharp representation of the membrane; pressure discontinuity over one computational cell was confirmed along a membrane not aligned with the computational mesh [3]. One example of sharp pressure distribution at the cylindrical membrane is shown in Fig. S2. For this case, both solute and solvent permeations are considered by including the coupling with osmotic pressure difference caused by mass concentrations [6].



(a)



(b)

Figure S2: Example of pressure distribution around a permeable membrane through which both solute and solvent are transported. (a) Schematic of the simulation setup and (b) steady pressure distribution $p(x, y)$ around a circular membrane fixed in a 2-D channel. The domain size is $H_0 = l = 3D_\mathrm{p}$, where D_p is the circle diameter, and the top and bottom walls are moved at a constant speed U_0. The pressure is shown normalised by ρU_0^2. The permeability is $\mathcal{L} = L_\mathrm{p}\mu/D_\mathrm{p} = 10^{-2}$, both the Reynolds and Peclet numbers based on U_0 and D_p are 1, the repulsion coefficient $\sigma = 0.5$, $\mu_\mathrm{L} = L_\mathrm{d}/L_\mathrm{p} = 1$ (with L_d being the phenomenological coefficients relating the diffusion flow to the osmotic pressure), and the pressure ratio of reference osmotic pressure to ρU_0^2 is $\mu_\mathrm{p} = 1$. See Ref. [6] for more detail.

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