Problem Statement

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1 Equations

In this section, we summarize the variables and partial differential equations that will be used to implement Physics Informed Neural Networks. The following convention is adopted from [2]. (Standard notation for space, time, velocity and pressure is used and not defined here.)

Specific terms for multiphase flows using the Continuum Surface Force approach [1]:

$$\sigma = \text{Surface tension coefficient}$$
$$\kappa = \text{Curvature of the interface}$$
$$n = \text{Surface normal of the interface}$$
$$\delta = \text{Dirac delta function (1 at the interface and 0 everywhere else)}$$
$$\phi = \text{Junction angle of the side channel relative to the main channel}$$
$$\alpha = \text{Volume Fraction}$$

Where,

$$n = \nabla\alpha$$
$$\hat{n} = \frac{n}{|n|} = \frac{\nabla\alpha}{|\nabla\alpha|}$$
$$\kappa = -\nabla\cdot\hat{n}$$

Variables used for non-dimensionalizing the conservation equations:

$$W_c = \text{Main channel width}$$
$$W_d = \text{Side channel width}$$
$$U_c = \text{Average inlet velocity in the main channel}$$
$$U_d = \text{Average inlet velocity in the outlet channel}$$
$$\mu_c = \text{Molecular viscosity of the continuous phase}$$
$$\mu_d = \text{Molecular viscosity of the dispersed phase}$$

The definitions of the non-dimensional variables:

$$x^* = \frac{x}{W_c}; \quad y^* = \frac{y}{W_c}; \quad u^* = \frac{u}{U_c}; \quad t^* = \frac{U_c}{W_c}t; \quad p^* = \frac{W_c}{\mu_c U_c}p; \quad \kappa^* = W_c\kappa; \quad n^* = W_c n$$

Bulk properties of the fluid are calculated as the volume weighted average of the two flows:

$$\rho = \alpha\rho_c + (1-\alpha)\rho_d$$
$$\mu = \alpha\mu_c + (1-\alpha)\mu_d$$

Non-dimensional conservation equations for the continuous phase (Star notation ($*$) is dropped from this point onwards):

$$\nabla\cdot u = 0$$
$$Re\left[\frac{\partial u}{\partial t} + (u\cdot\nabla)\,u\right] = \nabla\cdot\left\{-pI + \left[\nabla u + (\nabla u)^T\right]\right\} + \frac{1}{Ca}\kappa n\delta$$
$$\frac{\partial\alpha}{\partial t} + (u\cdot\nabla)\,\alpha = 0$$

Momentum Equation rewritten for the dispersed phase:

$$\gamma Re\left[\frac{\partial u}{\partial t}+(u\cdot\nabla)\,u\right]=\nabla\cdot\left\{-pI+\beta\left[\nabla u+(\nabla u)^T\right]\right\}+\frac{1}{Ca}\kappa n\delta$$

Where,

$$Re=\frac{\rho_c U_c W_c}{\mu_c};\quad Ca=\frac{\mu_c U_c}{\sigma};\quad \gamma=\frac{\rho_d}{\rho_c};\quad \beta=\frac{\mu_d}{\mu_c}$$

2 PDEs, IC and BCs in Cartesian form

The continuity equation can be represented as follows:

$$\frac{\partial u}{\partial x}+\frac{\partial u}{\partial y}=0 \tag{1}$$

The N-S equation for X -direction can be represented as follows:

$$\rho\left[\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}\right]=-\frac{\partial p}{\partial x}+\mu\left[\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right]-\sigma\frac{\partial \alpha}{\partial x}\nabla\cdot\hat{n} \tag{2}$$

Similarly, the N-S equation for Y-direction is:

$$\rho\left[\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}\right]=-\frac{\partial p}{\partial y}+\mu\left[\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right]-\sigma\frac{\partial \alpha}{\partial y}\nabla\cdot\hat{n} \tag{3}$$

Important: Please check the curvature formula Jupyter Notebook for the equation of the surface curvature ($\nabla\cdot\hat{n}$).

The convection-diffusion equation for the volume fraction

$$\frac{\partial \alpha}{\partial t}+u\frac{\partial \alpha}{\partial x}+v\frac{\partial \alpha}{\partial y}=0 \tag{4}$$

The initial conditions could be random, because we are interested in behavior after long time. (To be discussed)

For boundary conditions, the three inlets are provided with fully developed Poiseuille flow with the following average velocities. Additionally, extra terms have been defined.

$$U_c=1;\quad U_d=\frac{w_f}{2\lambda(1-w_f)};\quad w_f=\frac{Q_{d1}+Q_{d2}}{Q_c};\quad \lambda=\frac{W_d}{W_c}$$

The walls of the microfluidic channel are assigned with no-slip condition and pressure gradient in the normal direction as zero.

$$u=0;\quad v=0;\quad \frac{\partial p}{\partial n}=0 \tag{5}$$

For adjusting the normal of the interface near the walls, wall adhesion boundary condition is used. For this study, $\theta_{wa}=180$

$$\hat{n}=\hat{n}_{wa}\cos\theta_{wa}+\hat{\tau}_{wa}\sin\theta_{wa} \tag{6}$$

The outlet pressure is set to atmospheric.

$$p=0 \tag{7}$$

References

[1] J. Brackbill, Douglas Kothe, and Zemach CA. "A Continuum Method for Modeling Surface Tension". In: *Journal of Computational Physics* 100 (July 1992). DOI: 10.1016/0021-9991(92)90240-Y.

[2] Ich-Long Ngo, Sang Woo Joo, and Chan Byon. "Effects of Junction Angle and Viscosity Ratio on Droplet Formation in Microfluidic Cross-Junction". In: *Journal of Fluids Engineering* 138.5 (Jan. 2016). 051202. ISSN: 0098-2202. DOI: 10.1115/1.4031881. eprint: https://asmedigitalcollection.asme.org/fluidsengineering/article-pdf/138/5/051202/6195577/fe_138_05_051202.pdf. URL: https://doi.org/10.1115/1.4031881.