A Level Set Based Method to Simulate Contact Line Motion and Dynamic Contact Angles for Multiphase Flow

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Abstract: A two part levelset framework is developed to simulate the contact line motion on a wall. The first part resolves the ill-posed reinitialization problem for a signed distance function when a wall is present. The second is a microscopic forcing term to provide slip and force the contact angle to return to its static value at rest. The method shows good agreement to the analytic solution for the dynamic contact angle derived by Cox and experiments.

Keywords: Level set, contact line, multiphase flow in porous media

1 Introduction

Despite their abundance in nature, moving contact lines have presented a surprisingly complex numerical problem. One application where moving contact lines are particularly important is in the simulation of water transport in polymer electrolyte membrane fuel cells. In these devices, product water becomes trapped in the porous gas diffusion layer, effectively flooding the electrode and killing fuel cell operation. Standard interface techniques for multiphase fluid flow such as volume of fluid methods, front tracking techniques, and level set techniques do not take into account the contact angle of the fluids. This work aims to establish a framework using the level set technique to simulate accurately the motion of the contact line and predict the evolution of the dynamic contact angle.

2 Level Set Method

Although level set methods have been well established for their use with multiphase flows, there is comparatively little work on their use with a wall present. A signed distance function is traditionally used as the levelset function ϕ . However, this choice causes a problem when a wall is present since an entire region will fall outside of the domain of dependence of the characteristics in the Hamilton-Jacobi reinitialization equation (figure 1(a)). Several boundary conditions are proposed for the wall in the Hamilton-Jacobi equation and are tested for the translation of an angled wedge of fluid trapped between two plates with full slip. A zero-neumann boundary condition, the simplest choice, introduces errors to the simulation that drive the angle of the wedge towards 90° (figure 1(b)). If instead the angle is fixed to the value it had before reinitializing, no error is observed (figure 1(c)). In addition, this approach does not presume any dynamic contact angles and only preserves the existing angle.

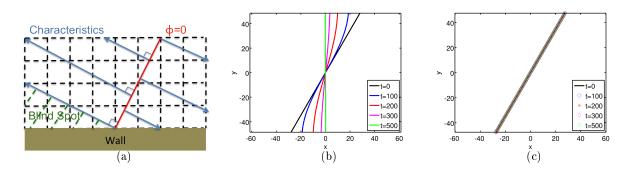


Figure 1: (a) Level set geometry showing the region outside the domain of dependence for reinitialization (blind spot). Interface evolution of the wedge for (b) zero neumann boundary condition (c) fixed angle boundary condition.

3 Microscopic Forcing Term

In order to drive the angle to its static contact angle, an additional forcing term is applied to the pressure jump condition in the ghost fluid method [1].

$$\frac{\Delta P}{\Delta y} = \sigma(\kappa + \kappa_{unr}) = \sigma\left(\kappa + \frac{\cos(\theta) - \cos(\theta_S)}{\Delta y}\right) \qquad (1)$$

This term can be derived as either an unresolved curvature or an unbalanced Young's force. When this force is used on a flow with no-slip at the wall, an apparent slip is generated. The results for the dynamic contact angle compare well with the analytic solution derived by Cox [2] and correspond to a realistic slip length (figure 2). Additional comparisons to experimental results for the dynamic contact angle for flow in a tube are shown.

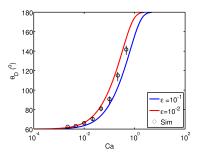


Figure 2: Comparison of numerical dynamic contact angles θ_D to predictions from Cox's asymptotic analysis for various capillary numbers Ca.

4 Conclusion

A new model for implementing a contact angle at the wall in multiphase flows is proposed. This model leads to good agreement with existing theory of the dynamic contact angle. Future work will investigate the possibility of additional friction laws at the contact line.

This material is based upon work supported by the National Science Foundation Graduate Research Fellowship under Grant No. DGE-1144469.

References

- R. Fedkiw, T. Aslam, B. Merriman, and S. Osher. A Non-osciallatory Eulerian Approach to Interfaces in Multimaterial Flows. J. Comp. Phys., 152:457-492, 1999.
- [2] R.G.Cox. Intertial and Viscous Effects on Dynamic Contact Angles. J. Fluid Mech., 357:249-278, 1998.