AN EFFICIENT COMPUTATIONAL MODEL FOR LARGE-SCALE SIMULATIONS OF MOVING CONTACT LINES

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Summary We propose an efficient level-set approach for numerical simulation of moving contact lines. The main purpose is to formulate, test and use a model wherein the large-scale flow is resolved whilst representing accurately the effects of the inner region around a contact line. Test simulations include both slow and fast droplet spreading on a flat surface. The results show that the present approach leads to excellent mesh convergence even with very coarse grids; furthermore, the results agree well with those obtained with a novel method for direct numerical simulations (wherein an adaptive grid is used).

INTRODUCTION

Many phenomena in nature and industry involve multiphase flows with moving contact lines, including any form of droplet spreading/impact on a solid surface. A major challenge in numerical simulation of moving contact lines is that the conventional hydrodynamic theory combined with a non-slip boundary condition leads to a non-integrable stress singularity at the contact line. In order to alleviate this stress singularity. The best documented method is that wherein the no-slip condition is replaced by a slip condition, thereby introducing a slip length parameter. Although the physical basis for slip remains unclear, theoretical results of such approach have been widely used and compare well with experiment. The fact that the slip length must be taken to be much smaller than other length scales in a flow remains a major hurdle in numerical simulations of these flows. In order to obtain mesh-convergent results, the slip length, which is usually nano-meter scale, must be resolved in direct numerical simulations of a slip-length-based method. In interface-capturing methods such as level-set [1] or VOF [2], an indicator function defined at the center of a computational cell is advected by a face-normal velocity, which induces numerical slip that tends to scale with the mesh size. The purpose of the present study is to develop and use an efficient approach in level-set method, to model the micro region near the contact line using Cox' theories [3, 4] and resolve the outer region, so that the macroscopic dynamics can be accurately captured with much reduced computational cost. The present approach is not limited to slow motion of moving contact lines.

NUMERICAL MODEL

Although the method proposed here is in principle of use generally, we use the important case of axisymmetric droplet spreading here as the main problem setup. The starting point of the level-set method used herein is essentially the method of [1], although a finite volume method based on a marker-and-cell (MAC) mesh is employed here. The velocity components are defined at cell faces and scalar variables such as pressure and volume fraction are defined at the cell centres. A fifth-order weighted essentially non-oscillatory (WENO) is employed in the discretization of the advection term in level-set function using the local flow velocity as the upwinding direction. In order to introduce the proposed model, it is necessary to first briefly review prior theoretical work of Cox. In Cox' viscous theory [3], which is valid for slow contact-line motion, the angle that the interface makes with the wall θ in an intermediate region follows

$$g(\theta, r_v) = g(\theta_w, r_v) + Ca\left(\ln\frac{d}{\epsilon}\right) + CaQ_i, \tag{1}$$

where $g(\theta, r_v)$ is defined in [3], θ_w is the wetting angle in inner region around the contact line, Ca is the capillary number based on the contact-line speed, r_v is the viscosity ratio, d is the distance to the contact line, ϵ is the ratio between slip length and a macroscopic characteristic length and Q_i is a constant depending on the inner slip model, r_v and θ_w. If instead the contact line moves fast (small values of $Oh = \sqrt{Ca/Re}$, where Re is based on drop radius and contact line speed), Cox [4] divided the intermediate region into a viscous intermediate sublayer where Eq. 1 applies and an inviscid intermediate layer. The interfacial angle, θ^* at the boundary of these two layers ($d = 1/Re$) follows from

$$g(\theta^*, r_v) = g(\theta_w, r_v) + Ca\left(\ln\frac{1}{\epsilon Re}\right) + CaQ_i, \tag{2}$$

whereas in the inviscid subregion

$$g_{iv}(\theta) = g_{iv}(\theta^*) + Ca\ln(Red), \quad Re^{-1} < d < 1 \tag{3}$$

In [1], the contact angle boundary condition is implemented at $0.5dr$ above the wall, and is set equal to the wetting angle in the inner region of the contact line. We propose here instead to determine the interfacial angle at this length scale from Eq. 1 or Eq. 3 in the case of slow or rapid spreading, respectively, and to use the interfacial angle $\theta_{num} = \theta(z = 0.5dr)$

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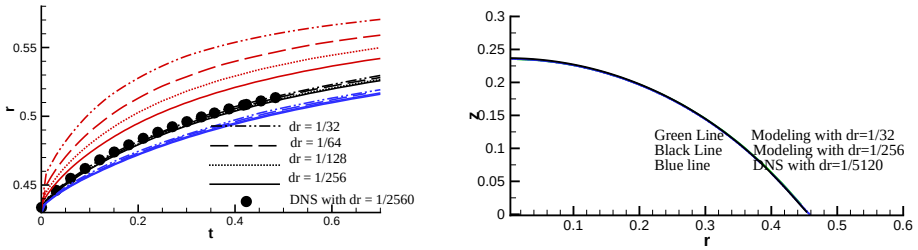

Figure 1. Axisymmtric droplet spreading on a flat surface with $r_v = 0.1$, $\lambda = 0.0001$,$\theta_w = \pi/6$ and $Oh = 0.1$. (a) contact line radius as a function of time. Red lines are for contant $\theta_{num} = \pi/6$. Black lines are for θ_{num} from Eq. 1. Blue lines are for θ_{num} from Eq. 1 with Q_i neglected. Black dots are for direct numerical simulation with adaptive mesh refinement. (b) instantaneous interface profiles from modeling and DNS.

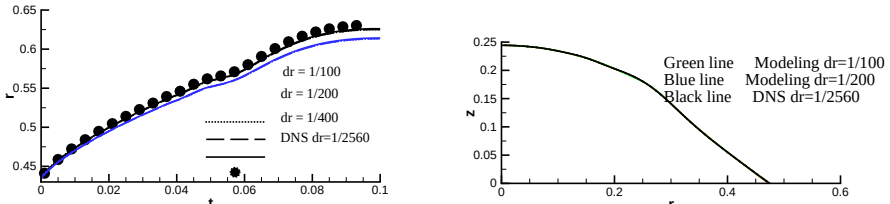

Figure 2. Fast axisymmtric droplet spreading with $r_v = 0.1$, $\lambda = 0.0001$,$\theta_w = \pi/6$ and $Oh = 0.00316$. (a) contact line radius as a function of time. Black lines are for θ_{num} from Eq. 1 or Eq. 3. Blue lines are for neglected Q_i. Black dots are for direct numerical simulation with adaptive mesh refinement. (b) instantaneous interface profiles from modeling and DNS.

as the contact angle boundary condition. At $z = 0.5dr$, d can be approximated by $z * cosec0.5[(\theta_w + \theta)]$. Special attention should be paid to cases where the contact line moves fast: one needs to first check which layer the interface at $z = 0.5dr$ falls in and then decides to use Eq. 1 or 3. To test the predictions we have carried out also direct numerical simulations. In order to simulate flows for realistic values of a dimensionless slip length, $\lambda = O(10^{-4})$ (normalized by drop diameter) at most, we have also incorporated into our method the free open-source software package, PARAMESH in a separate version of the code. This is an adaptive mesh refinement (AMR) tool developed for parallel computing.

RESULTS AND DISCUSSION

In Fig. 1 results are presented for slow axisymmetric spreading of $Oh = 0.1$. From Fig. 1a, the results represented by red lines, it is of course clear that when the grid spacing is significantly larger than the slip length, DNS with the contact angle set as the inner wetting angle cannot yield converged results; the drop spreads much faster than that from fine mesh simulation (we have tested and found $dr = 1/5120$ leads to converged results for $\lambda = 0.0001$). With the new model, it is seen (black and blue lines) that good mesh convergence is achieved even with a very coarse mesh. Furthermore, the modeling results using Eq. 1 (Q_i is obtained from [5]) with $dr = 1/32$ can compare well with those of the DNS with $dr = 1/5120$. We also find that neglecting the term Q_i, as had been done in most previous studies, leads to a quantitative difference and worsens the comparison with DNS. In Fig.1b, it is seen that the instantaneous drop shapes from the modeling with very coarse mesh agree well with DNS results with a mesh size that is two orders of magnitude smaller. Regarding the computation time, a simulation using the present approach with $dr = 1/32$ takes about 5 minutes on a single PC; while a DNS simulation with mesh grid size of $dr = 1/5120$ takes 140,000 cpu hours on the High-Performance Computing facility at Imperial College London, typically using 64 processors. A further test is for fast drop spreading with $Oh = 0.00316$. To our best knowledge, no such numerical model has been developed so far for similar situations where the contact line moves fast. From the results presented in Fig. 2, it can be seen that similar to the viscous model, the present inertial model also leads to good mesh-convergence performance and the modeling with coarse mesh agrees quite well with the grid-converged DNS results. From Fig.2b, it is seen that macro-scale dynamics like capillary waves traveling along the drop interface can be accurately captured with the present inertial model.

CONCLUSIONS

Within the framework of level-set method, we developed an efficient approach based on Cox' theories to model moving contact lines in both viscous and inertial regimes. Our model leads to good grid-convergence performance even with a very coarse mesh, and the results agree very well with DNS results wherein adaptive mesh refinement was used.

References

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