Numerical Simulation of the Spreading of Droplets

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Abstract

The fluid dynamical behaviour of thin liquid films, whether forced to spread over a solid surface or deposited/printed as a distinct pattern, is of enormous significance to manufacturing industry and practice. Such flows involve the presence of a free surface, dynamic wetting and interfacial phenomena such as surface tension gradients, each of which represents a considerable challenge in its own right. This paper describes the development and application of a novel, fast, state-of-the-art numerical algorithm for the solution of a particular class of governing fluid flow equations, generic to these types of free surface problem.

1. Introduction

The spreading of thin liquid films or droplets is ubiquitous [1-4] with applications ranging from the spreading of pesticides to the deposition of coatings or inks. This explains the wide interest in understanding the physics of spreading and particularly how it is affected by the presence of topographical and/or chemical heterogeneities. Such problems have been solved numerically by invoking a long wavelength approximation with the motion described by the lubrication equations. Schwartz and co-workers [6-10] have adopted a time-splitting approach for this purpose however the present work uses a multigrid strategy which has several desirable advantages [11] in terms of efficiency, accuracy and robustness. The solver in this case is fully implicit and unconditionally stable enabling the use of large time steps without loss of stability. In addition, the CPU time required to solve a discrete set of equations is simply proportional to the number of unknowns.

2. The mathematical model

The governing equations, first introduced by Greenspan [12], which describe the evolution of a droplet of height h(x,y,t) above a topography of height s(x,y) on a substrate inclined at an angle α, are in dimensionless form:

$$\frac{\partial h}{\partial t} = \nabla \cdot \left[\frac{h^3}{3} \left(\nabla P - Bo \sin \alpha \right) \right] \quad , \tag{1}$$

$$P = -\nabla^2 (h+s) - \frac{(n-1)(m-1)(1-\cos\theta_e)}{h^*(n-m)\varepsilon^2} \left[\left(\frac{h^*}{h} \right)^n - \left(\frac{h^*}{h} \right)^m \right] + Bo(h+s)\cos\alpha \ . \tag{2}$$

These equations are scaled with respect to R_0, a scaling droplet radius and the lubrication approximation assumes that if h_0 is the scaling drop height then $\varepsilon = h_0/R_0$ is small. The time is scaled by $T = \frac{\mu R_0}{\sigma \varepsilon^3}$ where μ is the viscosity and σ is the surface tension, and $Bo = \frac{\rho g R_0^2}{\sigma}$ is the Bond number. Here the fluid is Newtonian and surface tension is assumed constant. The second term in eq. (2) is the disjoining pressure term [6-9] used to alleviate the singularity at the contact line. This model assumes a thin precursor film of thickness h^* ahead of the contact line where *n* and *m* are the exponents of the interaction potential and θ_e is the contact angle at equilibrium. The governing eqs. (1) and (2) are discretized using finite differences on a uniform mesh subject to the boundary conditions of zero gradient for the height and for the pressure on the edge of the substrate. The numerical scheme used to discretize eqs. (1) and (2) is second order accurate in space and fully implicit first order in time [11].

3. Method of solution

Due to the non-linear nature of the problem, the method of solution employs the FAS (*Full Approximation Storage*) multigrid approach first introduced by Brandt in 1977 [14]. The set of discretized equations is solved on a hierarchy of grids (six in this case) in which the mesh size is halved from one grid level to the next finer one - the finest grid being 257*257. Quantities are transferred between grids using bilinear interpolation and a half-weighting

restriction operator. A *Red-Black Modified-Jacobi iteration* technique is used to smooth the errors on all but the coarsest grid level, those on the latter are solved using a Newton-Raphson iteration scheme. The efficiency of the *Multigrid* solver depends critically on the accuracy to which the equations are solved on the coarsest grid and, therefore, these are solved to a very small error tolerance.

4. Results

4.1. Droplet spreading on a uniform substrate in the absence of gravity

As a first validating case, a paraboidal droplet spontaneously spreading over a homogeneous horizontal substrate is considered, a problem that has been explored by others both experimentally in [1-3] and theoretically in [5,6]. Accordingly, the wetted area, πR^2 , is found to satisfy a power-law:

$$\pi R(t)^2 = KV^{\alpha} t^{\beta} \quad , \tag{3}$$

where V is the Volume of the droplet, α is typically 0.6 and $0.16 \le \beta \le 0.32$, [4], while Tanner [3], predicts that the maximum height of the drop, $\bar{h}$, is:

$$\bar{h} = \frac{K}{t^{0.2}} \quad , \quad t > 0 \, . \tag{4}$$

In the present study typical conditions are used, namely $h_0 = 2.10^{-5}$ m, $R_0 = 0.002$m, $\rho = 1000$ kg/m^3, $\sigma = 0.073$ N/m. Finally, the equilibrium contact angle θ_e is taken as 2.3° and the initial profile of the droplet is given by:

$$h(x, y, 0) = \gamma \left(1 - 4 \frac{\gamma}{\kappa} r^2 \right) \quad , \quad 0 \le r \le R \quad , \tag{5}$$

where γ, the ratio of the initial free surface height at the centre of the drop to the one at equilibrium and is set equal to 10. This choice of initial profile is convenient because it ensures that when the drop reaches its equilibrium position, it lies entirely on the substrate and is therefore captured within the computational domain.

Figure 1 shows the height at the centre of the droplet against time as a function of the precursor film thickness h^*. A log-log scale is used to show that the expected power-law is satisfied over a wide range ($10^{-8} < t < 10^2$). By fitting a curve of the type $\bar{h} = \frac{K}{t^{\beta}}$ in the linear region, β is found to be approximately 0.17, in good agreement with Tanner's value of 0.2-see eq. (4). The constant K varies slightly with the precursor film thickness and

ranges from 0.44 for h^* = 0.04 to 0.52 for h^* = 0.005. As in [6], it is found that an increase in h^* causes the droplet to spread more quickly. For example, increasing h^* from 0.005 to 0.04 increases the rate of expansion by 18%.

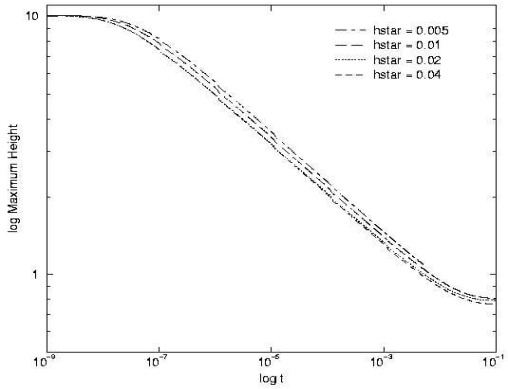

Figure 1: log-log plot of $\bar{h}$ versus t for different h^*

4.2. Effect of gravity on the levelling of a droplet over a topography

Orchard [15] used Fourier series to derive the time scale for the levelling of viscous liquids. Depending on the importance of gravity compared to surface tension, it is found that the corresponding levelling time scales, T_s and T_g, are given by:

$$T_s = \frac{3\mu R_0^4}{\sigma h_0^3} \text{ if } Bo << 1 \text{ ,} \qquad T_g = \frac{3\mu R_0^4}{\left(\sigma + \rho g R_0^2\right) h_0^3} \text{ if } Bo >> 1 \quad .$$

The following results demonstrate the ability of the solver to predict levelling over these widely different time scales. Figure 2 shows the drop profile at various times for an initially paraboloidal droplet lying on a high energy surface (θ_e = 0°) for *Bo* = 0. If the levelling ratio is defined as:

$$L_r = \frac{h_{\max}(t) - h_{\min}(t)}{h_{\max}(t_0) - h_{\min}(t_0)} \cdot 100 \quad , \tag{6}$$

when the dimensionless time reaches the Orchard levelling time scale T_s , a levelling ratio of 1.8% is found.

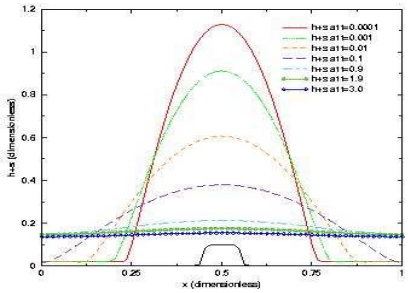

Figure 2: Drop profiles at various times, Bo = 0

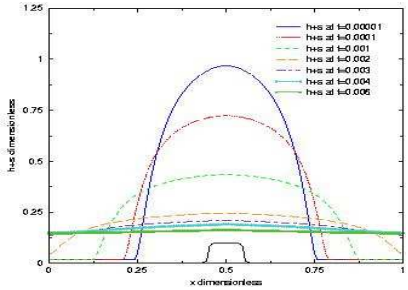

Figure 3: Drop profiles at various times, Bo = 950

For *Bo* = 950, Figure 3, when the time reaches the Orchard levelling time scale, the levelling ratio is: L_r = 2.8%. The numerical results agree well with the prediction of Orchard in both cases, where the effect of the gravity is to reduce considerably (by a factor of 950) the time necessary for the levelling of the droplet.

4.3. Efficiency of the solver

As mentioned previously, the main reason for using a *Multigrid* solver is its efficiency. The problem described in 4.1 was solved with a finest grid level of 33*33, 65*65, 129*129 and 257*257. The CPU time required in each case, for a single typical time step, is shown in Figure 4. It can be seen that the CPU time increases *linearly* with the number of unknowns, showing that the solver is operating at around its optimal efficiency.

5. Conclusion

This study describes an efficient and very stable numerical approach for solving the governing equations relevant to the spreading of thin liquid droplets. The Multigrid solver has been validated and results are consistent with previously-reported experimental and analytical results. The fine spatial

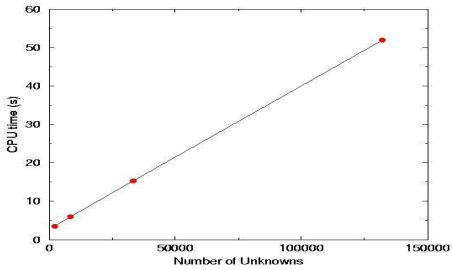

Figure 4: CPU time taken for a typical time step for different fine grid levels

resolution that is achievable efficiently with the Multigrid approach offers the potential to investigate more complicated flows, such as those over topographies and/or with steep property gradients. Improvements to the numerical scheme such as adaptive time stepping, to further increase its efficiency, and error control are currently ongoing.

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7. References

1. Hyppia, J., Anal. Chem., **20**, 1039 (1948)
2. Lelah, M. and Marmur, A., J. Colloid Interface Sci., **82**, 518 (1981)
3. Tanner, L., J. Phys. D, **12**, 1473 (1473)
4. de Gennes, P.G., Rev. Mod. Phys., **57**, 827 (1985)
5. Barenblatt, G.I., Berreta, E. and Bertsch, M., Proc. Natl. Acad. Sci. USA, **94**, 10024 (1997)
6. Schwartz, L.W. and Eley, R., J. Colloid Interface Sci., **202**, 173 (1998)
7. Eres, M.H., Weidner, D.E. and Schwartz, L.W., Langmuir, **15(5)**, 1859 (1999)
8. Schwartz, L.W., Langmuir, **14(12)**, 3440, (1998)
9. Weidner, W.E., Schwartz, L.W. and Eley, R.R., J. Colloid Interface Sci, **179**, 66 (1996)
10. Christov, C.I, Pontes, J. and Walgraef, M.G., Comput. Methods Appl. Mech. Engrg., **148**, 209 (1997)
11. Daniels, N., Ehret, P., Gaskell, P.H., Thompson, H.M. and Decre, M., Int. Conf. CFD Proceeding, 279 (2000)
12. Greenspan, H.P., J. Fluid Mech., **84**, 125 (1978)
13. Mitlin, V.S. and Petviashvili, N.V., Phys. Lett. A., **192**, 323 (1994)
14. Brandt, A., Mathematics of Computation, **31**, 33 (1977)
15. Orchard, S.E, Appl. Sci. Res. A, **11**, 451 (1961)