USING APPLIED MATHEMATICS IN INDUSTRIAL PROBLEMS

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1. Introduction

Traditional mathematics degree courses in Ireland have often placed the emphasis on the pure mathematics and even the applied courses offered have paid little attention to the possibilities for applying mathematics to real world problems. In the U.S., in Britain and in Europe, applied mathematicians have retained far stronger links with industry and the courses taught in the universities in these countries tend to be more closely attuned to the needs of the modern applied mathematician. This also means that mathematicians in these countries tend to be quite successful in their attempts at solving industrial problems and this, in turn, has led to mathematics obtaining more research funding from industrial sources than is the case in Ireland. I believe that we can redress this situation by a change in our approach to teaching applied mathematics in this country.

The applied mathematician in industry must, to some extent, be a jack-of-all-trades. The emphasis on teaching applied mathematics in Ireland has been placed on solving already formulated problems (for example, the student is presented with a differential equation and suitable boundary conditions), while the final "solution" will usually entail some complicated mathematical expression. The problem may be garnished with vague references to incompressible liquids/ cantilever beams, etc, but the emphasis is on solving the mathematical problem. The applied mathematician in industry realizes that solution of the formulated problem is only a small part of his overall task. In the industrial setting, he will typically be shown some experimental process and asked why it

does not work! This is a far cry from starting with a neat, properly formulated problem.

In my experience, formulation of the problem is possibly the most important step during the complex process of solving an industrial problem. A certain amount of basic physics is required, and at the very least the ability to communicate with physicists and engineers and ask them the right sorts of questions. Once the basic physics has been captured, for example by writing down a system of differential equations, physical insight is required to make reasonable simplifications without losing the essence of the problem. Then a full non-dimensionalization should be carried out leading (usually) to a reduction in the number of parameters in the problem (via the Buckingham Pi theorem) and the possibility for further simplification via asymptotic means by exploiting the occurrence of small parameters. At this point, the system can hopefully be analysed using asymptotic techniques or, if it is still too complicated, it can be solved numerically. Having attained solutions, the applied mathematician is certainly not yet finished. The (non-dimensional) solutions must now be interpreted to see what physical insight can be gained. Non-dimensional solutions often contain a wealth of physical information, but this has to be translated back into physics and suggestions made for improving the industrial process under consideration.

To summarize, the applied mathematician's approach to industrial problems can be divided into four steps:

- (i) formulation (physics to mathematics);
- (ii) simplification, non-dimensionalization of mathematical problem;
- (iii) analytical/numerical solution of mathematical problem;
- (iv) interpretation (mathematics to physics).

Traditional applied mathematics courses have concentrated on step (iii). Obviously a certain amount of physical intuition is required, and one extremely useful way of developing students' feel for physics is by including a *physical* fluid mechanics course at undergraduate level. This has the advantage that it is a subject rich in physical mechanisms (viscous effects, inertia terms, diffus-

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ive and convective phenomena) and approximations (slow creeping flow, thin film flow, boundary layer flow). It should certainly not be treated in a purely theoretical manner. Applied mathematics students should also be encouraged to take a certain number of physics courses and should be exposed to the elements of modelling and non-dimensionalization as early as possible. Finally, the basic *ideas* behind asymptotic methods (regular and singular perturbation theory) should be introduced as early as possible at an introductory level.

The rest of this article will consider a physical problem which I worked on at the Philips Research Laboratories in Eindhoven (in Holland), and illustrates the diversity of difficulties facing the industrial applied mathematician. In particular, while the formulation of the actual physical problem is carried out in Section 4 (followed approximately by steps (ii) to (iv) above), it should be noted that in order to reach this point a number of sub-problems must first be solved. Though this is not pursued in any detail here, each of these sub-problems also requires its own formulation, non-dimensionalization, simplification, etc.

2. Problem description

A dirt particle adhering to an integrated circuit (IC) decreases the stability and reliability of this IC. For ICs of current interest, particles of the order of $0.1\mu\mathrm{m}$ are critical. Existing cleansing methods (for example, scrubbing, jet cleaning) generally exert removal forces proportional to the surface area or volume of a dirt particle. Their success has been rather limited for particles of radius less than $1\mu\mathrm{m}$. The existence of such a lower limit may at first sight seem puzzling but can be explained by the fact that adhesion is caused primarily by:

$$F_A = \frac{AR}{6H^2}; \qquad H << R, \tag{1}$$

where F_A is the London-van der Waals force, A is the Hamaker constant, R is the particle radius and H is the gap between the particle and the substrate. During cleansing a force must be exerted on the particle which opposes the adhesion force. The methods

mentioned above exert a force proportional to the second or third power of the particle radius R. All other factors remaining the same, if we reduce the particle size then the forces of adhesion as in equation (1) will eventually dominate the removal forces. A cleansing technique which just succeeds for $R = 1 \mu \text{m}$ will fail when $R = 0.1 \mu \text{m}$. A new cleansing method is illustrated in fig.1. The substrate to be cleaned is immersed in water and as the dirt particle passes through the liquid/air phase boundary, the surface tension forces which originate at the contact line around the sphere can oppose the adhesion forces, given favourable wetting conditions (contact angles) i.e. conditions which result in a favourable removal force as denoted by F_{γ} . The crucial factor is that the capillary forces can be shown to be linear in R, so the method is essentially independent of particle size because the adhesion forces (1) which cause the particle to stick to the substrate are also linear in R. In the next section we summarize some of the experimental work done.

2.1. Experimental work

Precise details of the experiments are to be found in [2] and [4]. In summary, a number of silicon substrates were contaminated with TiO₂ (rutile), α -Fe₂O₃ (haematite) and SiO₂ (amorphous silica). Where necessary, the contaminated substrates were silylated to change the contact angles favourably. The substrates were then passed slowly through an air/water interface. Before and after immersion, the particles were sized and counted using an electron microscope. In general 70% – 97% of the particles were removed, given favourable wetting conditions. The method was equally successful for particles as small as 0.1 μ m provided the immersion velocity was in the range 1 μ m/sec to several cm/sec. Almost no particles were removed for velocities of the order of 10 cm/sec or higher.

3. Developing a mathematical model

Experiment suggests the existence of a critical velocity above which the removing process no longer works. We begin by ruling out gravity forces and hydrostatic pressure as being of any importance, since they will both be $O(R^2)$ or smaller and can

easily be shown to be negligible for particles of radius less than about 10 microns. The surface tension forces can be shown to be:

$$F_{\gamma} = 2\pi R \gamma \sin \phi \sin(\theta - \phi), \tag{2}$$

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 γ being the surface tension of a liquid-gas interface where we consider the situation depicted in fig.2 where the water level is rising. R is the radius of a dirt particle (assumed spherical), θ is the contact angle between water and the dirt particle and $\phi = \phi(t)$ indicates the position of the water/air interface at any time t. In fig.2 the net surface tension force F_{γ} clearly opposes the adhesion force F_A . In order to use (2) to write down the magnitude of the surface tension forces as a function of the time, it is necessary to solve a sub-problem which concerns the shape of the liquid free surface and involves finding an expression for ϕ as a function of time t. This is done in Section 3.1.

In what follows we assume constant contact angle. A full analysis of the problem would involve a Stokes' flow problem with its concomitant difficulties. Instead, we proceed in an adhoc fashion. It is probable that the solution to the problem lies in the occurrence of viscous effects which tend to oppose relative motion between the dirt particle and the substrate. In Section 3.2, we show how an expression for these forces can be found. We consider the situation represented in fig.2 as the fluid level rises. If at a particular point the resultant surface tension force (which in this case is wholly opposing the adhesion force) is greater than the adhesion force, the particle will tend to move away from the wall. Then, as in lubrication theory, we expect the generation of large viscous forces which offer great resistance to the further separation of sphere and substrate. It is not sufficient for the surface tension forces merely to be greater than the adhesion forces: this no longer guarantees removal. The viscous forces, which will presumably vary monotonically with the velocity of the particle, also retard its removal. Thus we require the particle to attain sufficient separation before the surface tension forces die away. As the particle starts from rest, we have

$$\int_{0}^{t} (F_{\gamma} - F_{A} - F_{\mu}) dt = mv(t), \tag{4}$$

where F_{μ} represents the viscous forces, and it becomes clear that the time for which the surface tension forces operate, and hence the velocity of fluid immersion, is crucial to ensure that the separation of the particle from the substrate is large enough, i.e. that the area under the curve (representing the impulse delivered to the particle) in fig.3 is as large as possible. We now propose a one dimensional model for a particle moving away from a substrate. Before we can proceed with formulating an equation of motion for the particle, we must first obtain expressions for the different forces acting.

3.1. Surface tension forces as a function of the time

The basic form of the surface tension forces is given by eqn (2) with $\phi = \phi(t)$, the form of ϕ being as yet unknown. We consider the situation occurring in fig.2 as the fluid level rises. The velocity at which the undisturbed meniscus at ∞ rises is constant but will not be the same as the rate of rise of the circle of contact on the sphere. The former is given by: $dh_{\infty}/dt = V$, where h_{∞} is the height of the water meniscus far from the particle (at ∞), i.e. the globally observed height. We thus view the dynamic formation of the meniscus as a series of quasi-steady state problems and seek a relationship between the undisturbed fluid meniscus height and the position of the contact line on the sphere as indicated by the angle ϕ or ϕ_0 (see fig.2).

We will not go into the details of solving this sub-problem here (see for example [3]), but the shape of the fluid meniscus is described by a non-linear ordinary differential equation and on non-dimensionalizing and exploiting the occurrence of a small parameter, ϵ ($\sim 10^{-3}$) which is the ratio between the particle radius R and the capillary length $a = (\gamma/\rho g)^{1/2}$, where ρ is liquid density and g is gravitational acceleration, we obtain a solution using matched asymptotic expansions and deduce the following relationship between the physical height, h (see fig.2), and the angle $\phi_0 = (\pi/2 - \phi)$, defining the position of the circle of contact as:

$$h = a\epsilon C(\ln \epsilon + \ln \left(\cos \phi_0 + \sqrt{\cos^2 \phi_0 - C^2}\right) - \ln 4 + \gamma_c), \quad (5)$$

where $C = \cos(\theta + \phi_0) \cos \phi_0$, γ_c being Euler's constant. As h is known as a function of t, so too is ϕ or ϕ_0 .

3.2. The viscous forces

As a particle starts to move away from the substrate (see fig.2), we expect the occurrence of strong viscous forces opposing the separation. In order to approximate this flow, we note that this so-called 'squeeze flow' between the sphere and substrate may be modelled using the lubrication approximation, as the layer of fluid separating the two bodies is so thin. We again neglect the details of this sub-problem. For the case in question where $H \ll R$, it was shown in [3] that the lubrication forces opposing separation

$$F = \frac{6\pi\mu V R^2}{H},\tag{6}$$

where V is the relative velocity between sphere and substrate. Thus the force required to effect separation is inversely proportional to the separation of sphere and substrate and directly proportional to the velocity of removal. Beer drinkers will have experienced similar 'squeeze flow' phenomena while trying to lift their glasses from a smooth wet table top!

4. Formulation, simplification, solution and interpreta-

4.1. Formulation

Referring to fig.2 we consider a force balance on a sphere moving away from the substrate, the sphere being considered a particle. Equilibrium occurs as result of a balancing of the inertial, surface tension, viscous and adhesion (van der Waals) forces on the particle. Then, considering eqns (1), (2) (incorporating (5)) and (6), we can formulate an initial value problem non-dimensionalized using the following scales:

$$x^* = \frac{x}{H}, \quad t^* = \frac{tV}{R},\tag{7}$$

where x(t) is the *separation* between sphere and substrate. We

thus formulate:

$$K\ddot{x}^* = G(t^*) - \frac{\delta}{(x^*)^2} - \lambda \frac{1}{x^*} \frac{dx^*}{dt^*},$$
 (8)

where

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$$G(t*) = \sin \left[\phi(Rt^*/V)\right] \sin \left[\theta - \phi(Rt^*/V)\right],$$

$$K = rac{2
ho_p V^2 H}{3\gamma}, \quad \delta = rac{A}{H^2 \gamma 12\pi}, \quad \lambda = rac{3\mu V}{\gamma} = 3Ca$$

and ρ_p is the density of the particle and Ca is the capillary number, while differentiation with respect to the time is denoted by a dot. As boundary conditions in dimensionless form we have:

$$x(0) = 1, \quad \dot{x}(0) = 0, \tag{9}$$

indicating that the particle starts form rest at a known distance from the substrate.

4.2. Simplification

Equations (8) and (9) can be considered a singular perturbation problem, as $K \ll 1$ (see also [3]). However it turns out that the outer solution obtained by solving eqn (8) ignoring the inertia terms and using only the first of the boundary conditions gives rise to a solution which also satisfies the second condition. Thus the problem does not display boundary layer behaviour at lowest order, and can be solved in closed form.

4.3. Solution

The solution of (8) satisfying the first boundary condition of (9) and neglecting the O(K) terms (this gives a Bernoulli equation) is easily shown to be:

$$x^{*2}(t^*) = \exp\left(\frac{2}{\lambda}[I(t^*) - I(0)]\right)$$
$$-\frac{2\delta}{\lambda}\exp\left(\frac{2}{\lambda}I(t^*)\right)\int_0^{t^*}\exp\left(-\frac{2}{\lambda}I(\theta)\right)d\theta,$$
 (10)

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where

$$I(t^*) = \int^t G^*(\tau) \, d\tau.$$

4.4. Interpretation

The important factor in (10) is the $2/\lambda$ which identifies the dimensionless group $\gamma/\mu V$ (as $\lambda=1/(3Ca)$), the reciprocal of the capillary number $Ca=\mu V/\gamma$, which has arisen naturally in the course of the analysis. The process of non-dimensionalization has indicated that the particular values of the surface tension γ , viscosity μ and velocity of immersion V are not in themselves important. Rather, the way in which they combine to form the capillary number Ca is what determines the dynamics of the motion. To optimize the process it is necessary to keep Ca as small as possible. (10) would traditionally have signified the end of the applied mathematician's work, but as pointed out in the introduction, the present phase is just as important.

In dimensional form the solution (10) becomes:

$$\begin{split} x^2(t) &= H^2 \exp\left[\frac{2\gamma}{3\mu R} \int_0^t F_\phi(\tau) d\tau\right] - \\ &\frac{2A}{36\pi\mu R} \exp\left[\frac{2\gamma}{3\mu R} \int^t F_\phi(\tau) d\tau\right] \int_0^t \exp\left[-\frac{2\gamma}{3\mu R} \int^\tau F_\phi(\upsilon) d\upsilon\right] d\tau \end{split}$$

where $F_{\phi}(t) = \sin \phi(t) \sin(\theta - \phi(t))$. In this instance the relevance of fig.3 can easily be seen. Decreasing the velocity of immersion increases the area under the surface tension-time graph and maximizes the separation between particle and substrate. Application of the results attained here to the physical problem (fig.1), which

makes the rather crude assumption that the meniscus is axisymmetric, in order to attain an estimate for the length of time for which the fluid meniscus remains in contact with the sphere (fig. 1; $\theta=\alpha=70^\circ$, $R=0.3\mu\mathrm{m}$, $\mu=10^{-3}\mathrm{kgm^{-1}s^{-1}}$, $A=1.5\ 10^{-19}\mathrm{J}$, $\rho=10^3\mathrm{kgm^{-3}}$), predicts a cut-off velocity of the order of 25cm/s. Above this value the process should no longer work, although experiment suggests that it is somewhat lower in the 10-15cm/s range.

5. Discussion of the physical model

There are a number of factors in the physical process which produce uncertainties in the results, e.g. the Hamaker constant A and initial separation H (see (1)). The latter is taken here to be 1nm but Kim and Lawrence, [1], suggest that a more realistic value would be 0.6nm. A further possible source of error is estimating when a particle is actually free from the substrate. As the nature of the van der Waals forces is known to change for a separation of 10nm, we arbitrarily assumed a particle to be free when it reached this distance, which is ten times the initial separation. Nevertheless the approximate model derived here captures the essential features of the experimental process, i.e. the significance of the viscous forces and the velocity dependent nature of the mechanism. One dynamic factor missing from the model is the variation of contact angle with substrate velocity for the simple reason that no values of the dynamic contact angle for the case considered in this paper are known, be it theoretically or experimentally. Leenaars [2] assumes that the contact angle remains constant.

The basic analysis identifies the capillary number as the most significant dimensionless parameter and indicates that the critical velocity of immersion can be increased by decreasing the ratio of μ/γ for the cleaning fluid. A further rather obvious improvement is also indicated: the experimental process as shown in fig.1 has the disadvantage that part of the removal power of the surface tension forces is lost due to the effect of the inclination α . The theoretical set-up in fig.2 removes this problem completely and results in a much higher theoretical critical velocity. In practice this arrangement would be difficult to obtain when dealing with

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submicron particles. However, a more favourable arrangement than fig.1 could be obtained by submerging the substrates at an angle, thus striving for a set-up between the extremes of figs.1 and 2. This also has the advantage of speeding up the process and of removing the uncertainty about the contact angle from the analysis.

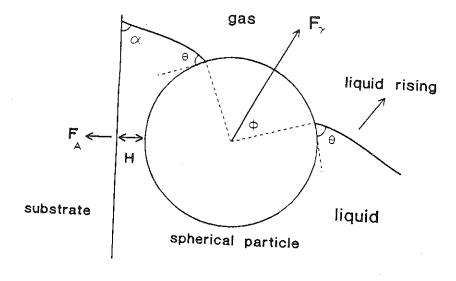


Fig. 1. Spherical particle adhering to substrate during passage of phase boundary.

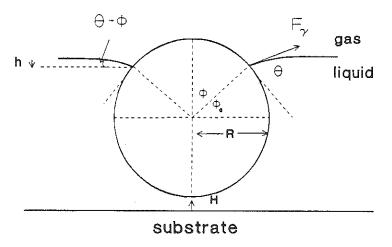


Fig. 2. Removal of particle from horizontal substrate.

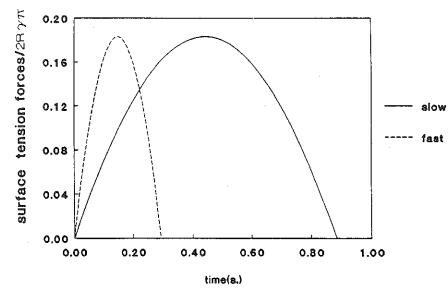


Fig. 3. Comparison of impulse delivered by F_{γ} for slow and fast immersion.

References

- [1] S. Kim and C. J. Lawrence, Chem. Eng. Sci. 43 (1988), 991-1004.
- [2] A. F. M. Leenaars, in Particles on Surfaces: Detection, Adhesion and Removal, ed. K. L. Mittal. Plenum: New York, 1988.
- [3] S. B. G. O'Brien and B. H. A. A. van den Brule , J. Colloid Interface Sci. 144 (1991), 210-222.
- [4] S.B.G. O'Brien and A. F. M. Leenaars , Philips J. Res. 44 (1992), 183-209.

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THE 35TH INTERNATIONAL MATHEMATICAL OLYMPIAD

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The International Mathematical Olympiad (IMO) is the most prestigious mathematical competition in the world for preuniversity students. It is held annually and the 1994 contest took place in Hong Kong in July. The number of countries and regions officially participating was 68. Each participating country sent a team of up to six members. The competition consisted of two four and a half-hour examinations, each exam made up of three problems. Each student competed as an individual and medals were awarded to the top performers.

IMO problems are celebrated for their extreme level of difficulty and some of them can even defeat professional mathematicians. It is no surprise, therefore, to find that a young student stands little chance of success in the competition, without a considerable amount of training. Some countries have a whole series of mathematics competitions—one for each year of the school programme-and in this way they can identify and encourage talented students from an early age. The first task in the process of choosing a team to represent Ireland in Hong Kong was to identify suitable candidates for training. Because a certain basis of mathematical knowledge is required in order to benefit from the training programme, generally only students who have completed the Junior Certificate are eligible. In November 1993 most secondary schools were invited to send up to three of their most mathematically talented pupils to attend training sessions in one of UCC, UCD, UCG and the University of Limerick. From information supplied by the Department of Education the top two hundred performers in the 1993 Junior Certificate mathematics examination were also personally invited to attend. The training sessions