Modeling of Coating Process for Production of Thin Films

Submitted to:

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Final Project Report
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Submitted by:

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Introduction

Coating processes find a wide variety of applications, including paints, membranes, photographic film, and semiconductor microelectronics. A thin film or films covering a large surface area of substrate necessitates coating of that film by some method. It is the motivation of this project to gain a fundamental understanding of the coating process by modeling the method of dip coating. Such significant quantities as the coating thickness variation and velocity profile may be predicted in terms of the final coating thickness, substrate velocity, and fluid properties.

Process Model

For the purposes of tractability of the proposed model, it will simplified as an infinitely long substrate (relative to the scale of the thickness) which is removed vertically with a constant velocity U from a pool of the fluid to be coated. The fluid is assumed to perfectly wet the substrate with a meniscus radius of curvature R. The final film thickness is δ_f. A diagram of the proposed model follows:

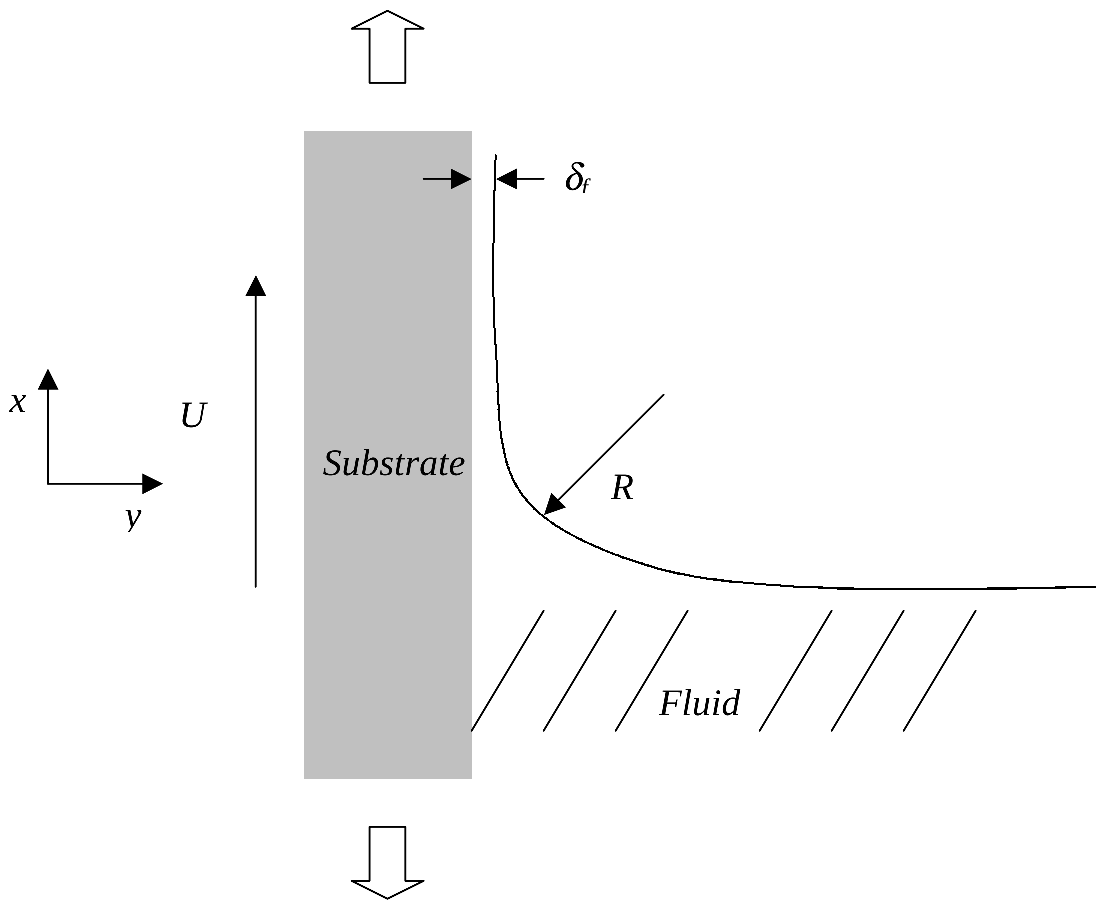

Figure 1: Diagram of Coating Process.

Assumptions

The following assumptions were made in the formulation of the model:

1. Surface tension forces dominate over viscous forces
2. Gravitational effects are neglected
3. The fluid completely wets the substrate.
4. The process is simplified as 2-D rectilinear flow.
5. The process occurs at steady state.
6. Inertial effects are neglected.
7. The lubrication theory approximation is used.

Model Formulation

We begin with the Navier-Stokes Equation:

$$\rho \frac{D\underline{u}}{Dt} = -\nabla p + \mu \nabla^2 \underline{u} + \rho g$$

In rectilinear coordinates, this becomes:

$$\rho\left(\frac{\partial u_x}{\partial t} + u_x \frac{\partial u_x}{\partial x} + u_y \frac{\partial u_y}{\partial y} + u_z \frac{\partial u_z}{\partial z}\right) = -\frac{\partial p}{\partial x} + \mu\left(\frac{\partial^2 u_x}{\partial x^2} + \frac{\partial^2 u_x}{\partial y^2} + \frac{\partial^2 u_x}{\partial z^2}\right) + \rho g_z$$

Using assumptions 2, 5, 6, and 7, this reduces to:

$$\mu \frac{\partial^2 u_x}{\partial y^2} = \frac{\partial p}{\partial x}$$

To determine the *dp/dx* term, the Young-LaPlace Equation is used:

$$\Delta p = -\gamma \nabla \cdot \underline{n} = -\frac{\gamma}{R}$$

where the curvature is as follows:

$$\frac{1}{R} = \frac{\partial^2 \delta(x)}{\partial x^2}$$

Substitution yields the following differential equation:

$$\boxed{\mu\frac{\partial^2 u_x}{\partial y^2}+\gamma\frac{\partial^3\delta(x)}{\partial x^3}=0}$$

with the No Slip and Free Surface boundary conditions:

$$u_x = U \; @ \; y=0$$

$$\tau_{xy} = -\mu\frac{\partial u_x}{\partial y}=0 \; @ \; y=\delta$$

The differential equation can now be integrated with respect to *y* at constant *x* to give the following result (complete derivation given in Appendix A):

$$\boxed{u_x(y)=U+\frac{\gamma}{\mu}\frac{\partial^3\delta}{\partial x^3}\left(\delta y-\frac{y^2}{2}\right)}$$

Now $\delta(x)$ needs to be determined to complete the derivation. To do this, the principle of conservation of mass is applied over the fluid film. The flow rate at any point along the film is equated to the final film flow rate:

$$\int_0^W\int_0^\delta u_x(y)dydz = U\delta_f W$$

where W is width of the film in the *z*-direction. This yields the following third order differential equation for $\delta(x)$:

$$\delta^3\frac{\partial^3\delta}{\partial x^3}+\left(\frac{3\mu U}{\gamma}\right)\delta=\left(\frac{3\mu U}{\gamma}\right)\delta_f$$

Analytical solution of this differential equation is facilitated by introduction of the following reduced dimensionless variables:

$$\bar{\delta}=\frac{\delta}{\delta_f} \qquad \bar{x}=\frac{x}{\delta_f}\left(\frac{3\mu U}{\gamma}\right)^{1/3}$$

Now the differential equation becomes, in terms of the reduced variables (see Appendix B for details):

$$\bar{\delta}^3\frac{\partial^3\bar{\delta}}{\partial\bar{x}^3}+\bar{\delta}=1$$

Using the following boundary condition:

$$\bar{\delta}\to \text{as} \;\; \bar{x}\to\infty$$

the differential equation reduces to:

$$\boxed{\frac{\partial^3\bar{\delta}}{\partial\bar{x}^3}=1-\bar{\delta}}$$

A solution to this differential equation follows:

$$\bar{\delta}=1+A\exp\left(-\bar{x}\right)=1+\exp\left(-\bar{x}\right)$$

where A is arbitrarily chosen to have a value of unity since it has no effect on the reduced thickness. Also, any exponentially increasing terms have been eliminated such that the solution is bounded. Finally, in terms of the original variables:

$$\boxed{\delta(x) = \delta_f\left[1 + \exp\left[-\frac{x}{\delta_f}\left(\frac{3\mu U}{\gamma}\right)^{1/3}\right]\right]}$$

Taking the appropriate partial derivatives and substituting into the equation for velocity (see Appendix C for details):

$$\boxed{u_x(y) = U - \frac{3U}{\delta_f^2}\exp\left[-\frac{x}{\delta_f}\left(\frac{3\mu U}{\gamma}\right)^{1/3}\right]\left[\delta_f\left(1 + \exp\left[-\frac{x}{\delta_f}\left(\frac{3\mu U}{\gamma}\right)^{1/3}\right]\right)y - \frac{y^2}{2}\right]}$$

And so the desired relationships for coating thickness and velocity profile have been determined.

Discussion

The final results give a good understanding of the scale of the coating thickness and velocity profile. However, a more useful result would require the determination of the final film thickness, δ_f. This requires another boundary condition. A possible methodology would be to divide the film into two regions: one for large *x* and one for small *x*. The results for the former region were developed above. The small-x region would require solution of another differential equation, which might only be done by numerical methods. The final boundary condition would then be to equate the curvatures of the two regions at the interface.

References

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3. Ruschak, K. J. *Limiting Flow in a Pre-Metered Coating Device*. Chemical Engineering Science, 1976