Numerical Simulation of the Dip Coating Process with Wall Effects on the Coating Film Thickness

Mahyar Javidi, Andrew N. Hrymak
Department of Chemical and Biochemical Engineering, Western University, London, ON, Canada

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The dip-coating process for the deposition of a liquid film on a cylindrical substrate is numerically simulated and wall effects of coating bath on the film thickness are investigated. In the present work, the hydrodynamics of non-Newtonian liquid films on cylindrical substrates is investigated with Carreau and powerlaw models. The method for determining the free surface is described including density, viscosity, surface and interfacial tensions considered.

Introduction

Vertical withdrawal of a substrate from a Newtonian or non-Newtonian pool of liquid, known as dip coating or free coating, is the oldest and the simplest coating method. Dip coating, as a popular post-metered coating method, is essential for the surface engineering of high-quality products. It is one of the better developed ways to enhance and alter the physical and mechanical surface characteristics. For instance, the performance properties of optical fibers, including abrasion resistance and strength, are strongly influenced by adding a coated layer. In recent years electro-active polymers have attracted much attention because of their great potential as actuators and sensors, and the cylindrical geometry may bring specific advantages to actuator design [1]. Therefore, cylindrical micro fabrication is of interest, in part, because of the advantages conferred by the substrate's shape. Unlike planar substrates, cylindrical substrates offer axisymmetric flexibility, complete surface area utilization, and radial symmetry. These unique properties offer opportunities such as catheter-based electronics in the medical industry, fiber optic modulation for medical devices, or equipment for heat and mass transfer in gas–liquid systems to provide a large interfacial area [2].

Landau and Levich [3] and Derjaguin [4] studied the liquid film formed on a moving flat plate and derived the film thickness expression at small capillary numbers. However, considering a film on a highly curved surface, where the radius of curvature of the wetted surface is in the order of magnitude of the film thickness the film flow can no longer be approximated by a planar liquid film. In addition to handling curvature effects, considering non-Newtonian fluids makes analytical calculation very complicated for cylindrical geometries. Knowledge of the relationship between the final coating thickness, withdrawal speed and fluid properties is essential for effective design, optimal control, and efficient operation of the free coating process.

Numerical Procedure

Simulation of dip coating process

Numerical solution for the incompressible Navier–Stokes equations with an Eulerian method is used. The mesh is treated as a fixed reference frame through which the fluid moves. In this work OpenFOAM used as CFD platform and volume of fluid (VOF) method is applied for capturing interface in the system [5, 6]. In the VOF method, the free surface, expressed by the volume fraction of one phase (e.g. α_1, for liquid phase), can be calculated by solving the continuity equation

$$\frac{\partial \alpha_1}{\partial t} + \nabla.(\alpha_1 u) = 0 \qquad (1)$$

However, in this method, the material discontinuity across the moving free surface is poorly described, resulting in a smeared free surface depending the local mesh density. To overcome this problem in obtaining a sharp interface, a method introduced by Rusche [7] in which an artificial surface compression term is added to the interface continuity equation leads to a sharper interface between the two phases.

$$\frac{\partial \alpha_1}{\partial t} + \nabla.(\alpha_1 u) - \nabla.(\alpha_1(1-\alpha_1)u_{r\alpha}) = 0 \qquad (2)$$

Where $u_{r\alpha}$ is the compression velocity given by

$$u_{r\alpha} = \min\left(C_\alpha |u|, max_G |u| \frac{\partial \alpha_1}{|\partial \alpha_1|}\right) \qquad (3)$$

Which tracks only the liquid surface due to α_1(1- α_1), whereby $\max_G|u|$ is the global maximum value of the velocity field. In addition, the momentum equation was solved with these mixture flow variables and surface tension is considered as an additional body force.

$$\frac{\partial \rho_f u}{\partial t} + \nabla.(\rho_f uu) = -\nabla P_{rgh} - (g.x)\nabla \rho_f + \nabla.\tau + \sigma k \frac{\partial \alpha_1}{|\partial \alpha_1|} \qquad (4)$$

For the numerical solution, the PIMPLE algorithm is used which is the combination of the PISO and the SIMPLE algorithms [5].

Results and Discussion

Numerical simulations have been completed for Newtonian fluids and non-Newtonian fluids. In the simulation, the physical properties of mineral oil were used for the Newtonian fluid and physical properties of 0.75% W solution of Polyox 301 in water used for the non-Newtonian fluid numerical calculations. Corresponding values for physical properties are shown in Table 1-3. For Carreau model, equation 6, was applied as the constitutive equation.

$$\mu = (\mu_0 - \mu_\infty)[1 + (\lambda\dot{\gamma})^2]^{\frac{n-1}{2}} + \mu_\infty \qquad (6)$$

In addition, for power-law model, equation 7, was considered as the constitutive equation.

$$\mu = (\kappa\dot{\gamma}^{(n-1)})\dot{\gamma} \qquad (7)$$

Newtonian fluid		
σ	ρ	μ
0.0284 N⁄m	876 kg⁄m^3	0.22 kg/m.s

Table 1**.** Physical properties of mineral oil

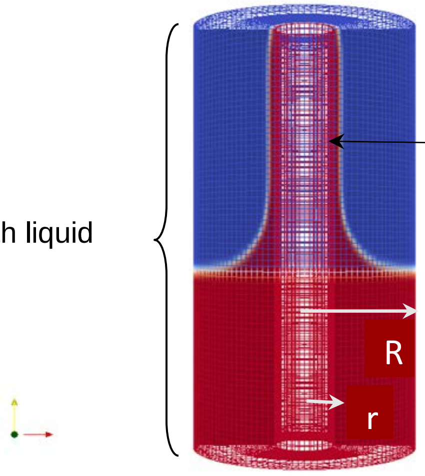
Power-law fluid			
σ	ρ	n	κ
0.062 N⁄m	1003 kg⁄m^3	0.64	0.066 (kg/m.s).s^n

Table 2. Physical properties of 0.75% W solution of Polyox 301 for power-law fluid

Carreau fluid					
σ	ρ	n	λ	μ_0	μ_∞
0.062 N⁄m	1003 kg⁄m^3	0.72	433.55	2.28	0.00

Table 3. Physical properties of 0.75% W solution of Polyox 301 for Carreau fluid

The final film thickness was considered at various withdrawal velocities and wall effect considered by applying the factor of (R/r) which is coating bath radius over the cylindrical substrate radius. Considering this factor in the free coating process can help getting uniform productions when high productivity is required, as in every industrial process. The domain sketch is illustrated in Fig 1.



Cylindrical substrate

Coating bath with liquid

Fig 1. Simulation of dip coating process including wall effect (In this picture two phases including gas (blue) and liquid (red) and the interfacial region shown in white)

Simulations have been prepared in three dimensions for capturing the accurate results and final film thickness was calculated at different withdrawal velocities which illustrated in Fig 1-3 for Newtonian, power-law and Carreau fluids respectively.

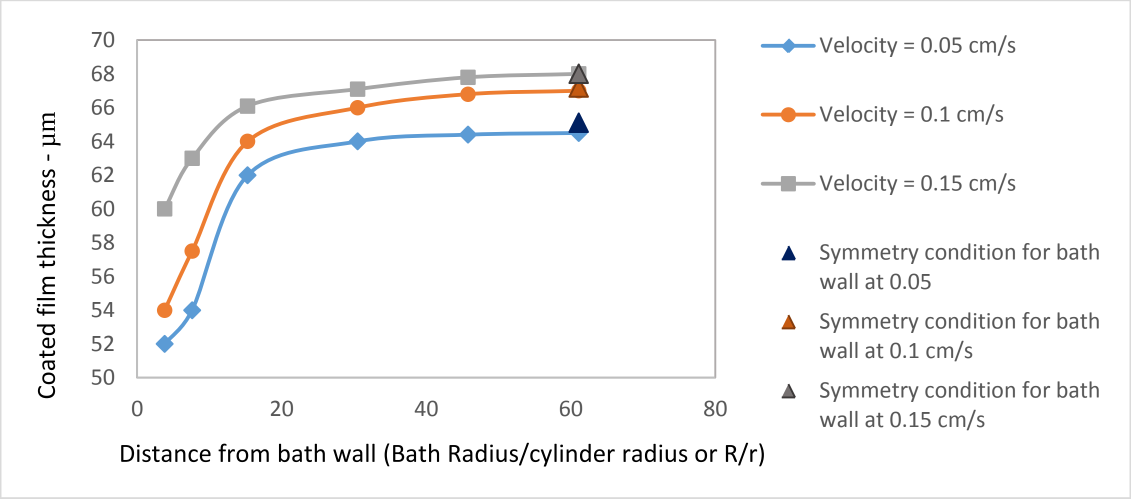


Fig 1. Coated film thickness vs. distance from coating bath wall for Newtonian fluid

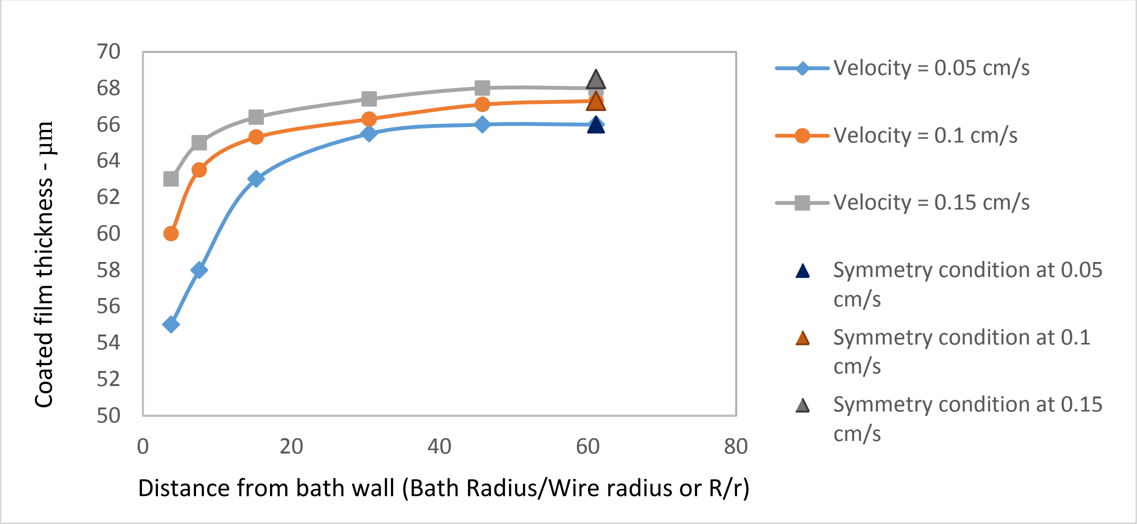


Fig 2. Coated film thickness vs. distance from coating bath wall for power-law fluid

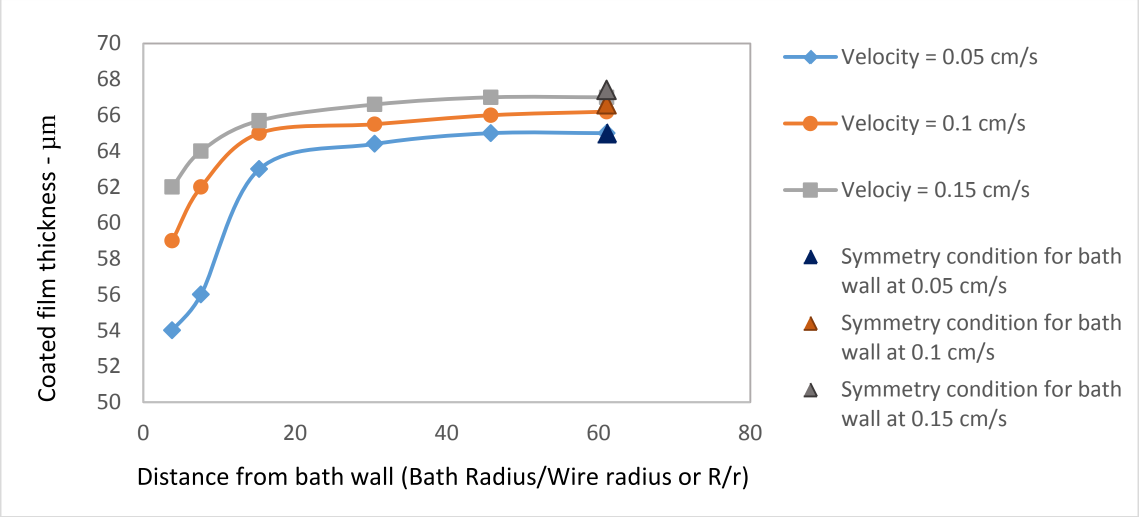


Fig 3. Coated film thickness vs. distance from coating bath wall for Carreau fluid

In all three models, the film thickness rises by increasing the ratio of R/r, however, for the values higher than around 30 for R/r, coated film thickness approaches a plateau value in relation to withdrawal velocity.

For R/r < 30, the bath wall plays a role similar to a die and results in a thinner film layer on the substrate. For R/r > 30 the film thickness approaches a plateau value as a function of withdrawal velocity and film thickness reaches the value calculated for infinite bath size by considering the symmetry condition for bath wall which achieved by applying zero gradient condition at the bath wall for velocity and bath level. The values of x-axis in Fig 1-3 are the actual values of R/r simulated in OpenFOAM.

Conclusion

The desired final thickness is affected by controlling the withdrawal velocity, material physical properties, substrates geometry and wall proximity. Simulation of dip coating process, regarding the wall effect has been completed in this work and confirms that the wall influences the coating thickness.

Reference

[1] A. Yang, X. M. Tao, X. Y. Cheng, Prediction of fiber coating thickness via liquid-phase process, Journal of Materials processing Technology, 202: 365-373, 2008
[2] J. Grunig, T. Skale, M. Kraume, Liquid flow on a vertical wire in a countercurrent gas flow, Chemical Engineering Journal, 164: 121-131, 2010
[3] L. Landau, B. Levich, Dragging of a liquid by a moving plate, Acta Phusicochim, 17:42-54, 1942
[4] B. Derjaguin, On the thickness of the liquid film adhering to the walls of a vessel after emptying, Acta Physicochim, USSR 39:13-16, 1943
[5] The OpenFOAM® Foundation
[6] C. Hirt, and B. Nicholls. Volume of Fluid (VOF) Method for Dynamics of Free Boundaries. Journal of Computational Physics, 39(1):201-225, 1981
[7] H. Rusche, Computational Fluid Dynamics of Dispersed Two-Phase Flows at high phase fractions. Ph.D. thesis, University of London, 2002