Current State of Theoretical Modeling of Coating Flows

J. M. de Santos [†], **M. S. Carvalho**[††], and **L. E. Scriven** [†]

† Department of Chemical Engineering & Materials Science
University of Minnesota, Minneapolis, MN 55455

†† Department of Mechanical Engineering
Pontificia Universida Catolica do Rio de Janeiro, RJ, Brazil

Presented at the 13th International Coating Science and Technology Symposium, September 10-13, 2006, Denver, Colorado[1]

Introduction. The viscous free surface flows in coating processes are complex enough that the systems of equations that describe them, whether the liquid is Newtonian or deformation rate-sensitive, cannot be solved by conventional mathematics. They require modern computer-aided functional analysis, or the older finite difference approximations or their descendants, a growing assortment of which is available in commercial and governmental software packages. They also require modern computers, of which laptops and desktops more frequently suffice but workstation clusters and supercomputers are often advantageous.

Minnesota experience. After over 30 years of research, development, and transfer to codes marketed to users who range widely in experience, the goal of comprehensive theoretical modeling is approached only in the combined abilities of the decidedly uncommercial research codes at U. Minnesota and PUC-Rio de Janeiro. Notwithstanding their lack of transportability and reliability, these codes stand as a beacon, because their development has not been circumscribed by incentives to cater to a wide range of customers many of whose needs diverge from steady, laminar, mostly two-dimensional coating flows and the transients, frequency response to ongoing disturbances, and stability to small episodic perturbations of these flows. Here we outline the research codes' nature in terms of their standard operating procedure.

Salient features of that procedure are Galerkin's and related methods of solving the governing equations; solutions expressed in finite element basis functions on elements defined by a mesh — neither

---

[1] Unpublished. ISCST shall not be responsible for statements or opinions contained in papers or printed in its publications.

Eulerian, Lagrangian, nor arbitrary — inscribed on an ether governed by rational transport or elastic domain deformation equations; coefficients of the basis functions found by solving their nonlinear algebraic systems efficiently with Newton iteration; reliable initialization of Newton iteration by potent continuation techniques; parsimonious probing of parameter space by continuation in parameters; evaluation of transient behavior, of frequency response to sinusoidal disturbances, and of stability to small perturbations, all by local linearization, eigenproblem reduction and efficacious solution; feature tracking, attenuation factor tracking, fold tracking and other critical point tracking by efficiently solving augmented systems of equations; and exploitation of these capabilities to analyze and troubleshoot coating flows, to design control systems to reduce coating variability, and to optimize applicator configuration and operating conditions with respect to defects induced by coating speed and other operating parameters as well as those induced by applicator shape design.

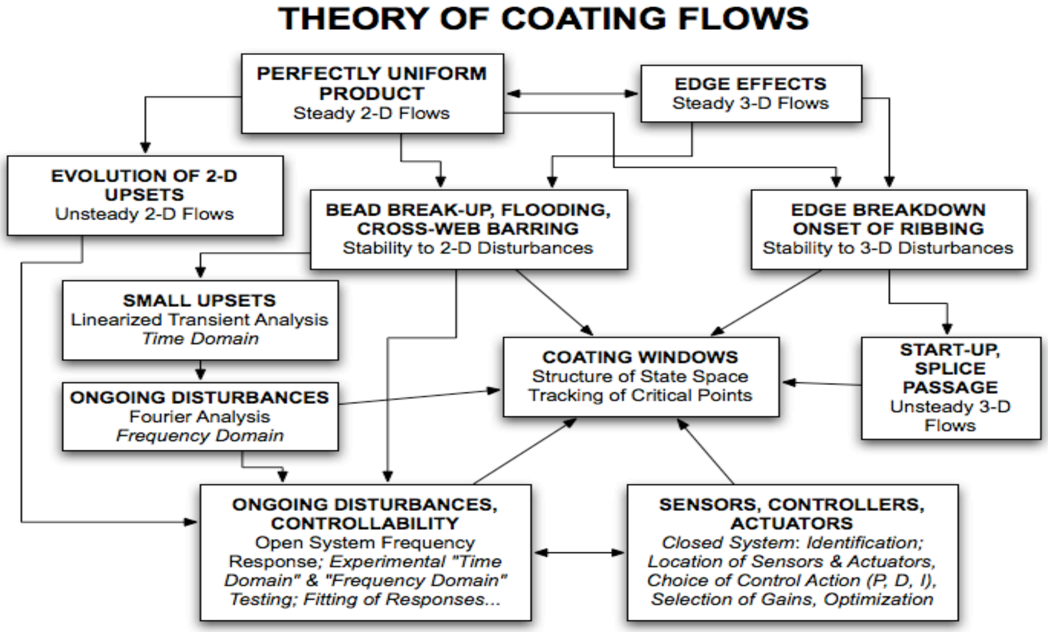
A solution is not enough! For purposes of design, control, and optimization, a solution, an operating state, is not enough. *Many* solutions are needed, even in the most parsimonious probing of parameter space. Many solutions are needed in order to get an idea of the ranges of design parameters and operating parameters within which steady, two-dimensional flow states exist. The final Jacobian matrix of sensitivities from each use of Newton's method makes it possible to proceed efficiently through parameter space, because that matrix makes it feasible to employ the scheme of first-order continuation in parameters. Arc-length continuation makes it possible to identify the limits of existence of steady, two-dimensional flow states when these limits are critical points (e.g. turning points, bifurcation points), as they often are. Arc-length continuation makes it possible also to find when more than one such flow state exists, a not uncommon situation, and the relative stability of the multiple states. Augmented continuation schemes make it possible to track critical points themselves through parameter space, e.g. turning points in a procedure called fold-tracking. This procedure can be used for delineating windows of feasible operation.

Within a feasibility window lie coating quality windows defined by features and sensitivities of the flow states, as already noted. Similar augmented continuation schemes make it possible to track through parameter space the limiting states at which a microvortex appears or disappears, a static contact line pins to an edge or moves free, and so forth — and in addition how the feasibility and quality windows depend on shape and dimensions of the coating die.

It is vital to know how sensitive the coated layer or layers delivered by an operating state are to disturbances. Disturbances in liquid flow come from the supply pumps; in substrate speed, from the drive mechanisms; in pressure difference, from fan fluctuations and sound waves; in gap, from substrate waviness, roll run-out, and mechanical vibrations, and so on. The Jacobian matrices of sensitivities make it possible easily to determine the responses to ongoing, sinusoidal, small-amplitude disturbances of given frequencies. To get these frequency responses, all that is needed is to solve, with GFEM, the linearized version of the Navier-Stokes system that describes the fully developed, sinusoidally varying flow. The Jacobian matrix of sensitivities also makes it possible to determine the normal modes of response to small-amplitude disturbances, spontaneously arising ones as well as imposed ones, and to compute the rates at which the most dangerous of these modes are damped or amplified in time. To get this stability information, it is necessary to solve a closely related, asymmetric, generalized eigenproblem for the ten or so leading modes, i.e. those whose eigenvalues have the largest real parts. Once these are computed, frequency response can be found, or at least interpreted, more efficiently by modal analysis, in which each sinusoidally varying imposed disturbance is decomposed into the leading modes plus a residue. Frequency response and stability information is pre-requisite to selecting active control schemes to reduce sensitivities and counter instabilities — an approach well-known elsewhere in technology but for coating flows quite challenging.

Quality windows are also delineated by set values of the damping coefficients and attenuation factors computed in stability and frequency analysis. These too can be traced out efficiently in parameter space by augmented continuation schemes. The same is true of the turning points and bifurcation points in parameter space, points defined by vanishing of the real part of an eigenvalue. These are the guides to situations in which there is more than one stable operating state. When these situations arise, it becomes desirable to solve repeatedly the full Navier Stokes system for time-varying flow in order to know how different start-up procedures and upsets select among the multiple stable states.

Fold-tracking, feature-tracking, stability and frequency analysis, and transient analysis are all tools for process design, control, and optimization. All of them we have demonstrated in conjunction with the computational fluid mechanics of coating flows. In our experience the Jacobian matrix needed for Newton iteration to compute each solution, or operating state, is a treasure trove. It is the key to sensitivity, stability, frequency response, and controllability — things just as important to know as the solution itself. It is also the key to continuation schemes with which parameter space can be probed with as small a number of solutions and their properties as are warranted by the practical objectives and the computational costs. This is what is meant by parsimonious probing. It is surely crucial to optimization of the design and operation of not only liquid coating, but also of other processes and equipment that are no less complicated.



REFERENCES

Benjamin, D. F. 1994. *Roll Coating Flows and Multiple Roll Systems*. Ph. D. Thesis, Univ. of Minn. Available from University Microfilms International, Ann Arbor, MI.

Christodoulou, N. C. & Scriven, L. E. 1992. Discretization of free surface flows and other moving boundary problems. *J. Comput. Phys*. **99**; 39-55.

Christodoulou, N. C. & Scriven, L. E. 1998. Finding leading modes of a viscous free surface flow: An asymmetric generalized eigenproblem. *J. Sci. Comput*. **3**: 355-406.

de Santos, J. M. 1991. *Two-Phase Cocurrent Downflow Through Constricted Passages*. Ph. D. Thesis, Univ. of Minn. Available from University Microfilms International, Ann Arbor, MI.

de Santos, J. M., Benjamin, D. F. & Scriven, L. E. 1992. Meshes as Solutions to Elliptic PDE's of Transport. AIChE Summer National Meeting, Minneapolis, MN, 9-12 August 1992.

Kistler, S. F. & Scriven, L. E. 1983. Coating Flows. In *Computational Analysis of Polymer Processing*, Chapter 8, pp. 243-299. Eds. J. A. Pearson & S. M. Richardson. London: Applied Science Publishers.

Kistler, S. F. & Scriven, L. E. 1984. Coating flow theory by finite element and asymptotic analysis of the Navier-Stokes System. *Int. J. Num. Meth. Fluids* **4**: 207-229.