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13. ABSTRACT *(Maximum 200 Words)*

The research produced accomplishments and new findings in the areas of thermomechanics and stability of materials with temperature-dependent density, characterization of pesticide spray solutions in agriculture and polymer solutions and melts in manufacturing, criteria for admissible forms of non-Newtonian viscosity for flows with low strain rates, modeling of industrial filament manufacturing processes, modeling fiber drawing and belt power transmission, material characterization in high strain-rate plasticity, and modeling of foam generation and flow. As an outgrowth of the research, the PI has collaborated with Prof. Palazotto of AFIT in two AFRL/DAGSI proposals, in response to topics generated by the Air Vehicle Directorate of WPAFB. One past the first cut and is currently being considered for funding.

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Final Technical Report for AFOSR No. F49620-97-0003, "Fluid Mechanics and Rheology of Liquid Fiber Flows: Fundamental Science and Technological Applications"

Progress during the period 01 August 1996 - 31 October 1998

P.I. Stephen E. Bechtel
Applied Mechanics, Ohio State University

Accomplishments/New Findings

For the purposes of this report I have separated the research effort into seven areas, noting that all are interrelated.

1. Thermomechanics and stability of materials with temperature-dependent density

This project originated with my work with Hoechst Celanese Corporation modeling the melt spinning of polyester fibers. Thermally induced shrinkage is an important feature of this process, and the state-of-the art modeling of the effect was a posteriori insertion of a temperature-dependent density function into the equations governing an incompressible fluid. In [2] we showed that this approach is thermodynamically inconsistent (it violates the second law), and derived, through the theory of a thermomechanically constrained material, a model which does not violate the second law. When applying this thermomechanically consistent model to pipe flows in that paper and [1], we predicted features qualitatively different than the commonly employed ad hoc model, in agreement with predictions based on the fully compressible theory.

We have applied the theory to fiber melt spinning [15], and predicted phenomena that are missed by the thermodynamically inconsistent theory. We have been able to derive the equations of our constrained theory also as a limiting case of a compressible material. In a startling development, Qi Wang found that a Newtonian fluid with temperature-dependent density and viscosity governed by our theory has a linearly unstable stress-free rest state. This has led us to study some interesting questions:

- If a small perturbation is driven away from the rest state, where does it go (to a neighboring small amplitude oscillation, to a static, stressed configuration, or far away from the rest state)?
- Are the steady state pipe flow and fiber spinning solutions we display in [1, 2, 15] stable?
- Most importantly, *is a stable rest state a necessary condition for a model* (said differently, does the fact that our theory has an unstable rest state make it an unphysical, unacceptable model)?

We have found in our literature search and discussions with researchers in the rational mechanics community concerned with the development of theories that this last question is open: The only criteria are that the theory must be consistent with invariance requirements under superposed rigid body motions and the second law. *There have been no stability requirements.* Further, in investigating this question we made a far-reaching discovery: Instability of the rest state is not special to our particular theory for a Newtonian fluid; *it is shared by any theory which postulates the constraint of temperature-dependent density,*

$$\rho = \rho(\theta). \tag{1}$$

Our work therefore led us in [13] to a reinterpretation of the thermal expansion coefficient α, a fundamental concept first introduced to students in high school physics. The current notion of the thermal expansion coefficient is tied directly to the constraint (1),

$$\alpha \equiv \frac{d\rho(\theta)}{d\theta}, \tag{2}$$

at some reference temperature θ_{ref}, and hence unavoidably brings with it instability of the rest state. Although it has not been checked in the past, stability of the rest state must be a necessary condition for a model, so that the constraint (1) is not allowed. The challenge therefore is to repair the the fundamental concept of thermal expansion by replacing (1) with a stable constraint. We have found in [13] that the constraint

$$\rho = \rho(\eta), \tag{3}$$

where η is entropy, yields a stable rest state. A repair of the thermal expansion coefficient is that α is actually

$$\alpha \equiv \frac{d\rho(\eta)}{d\eta}, \tag{4}$$

and that experiments used to characterize α have been performed under reversible conditions in which the entropy path can be deduced from the temperature path. A proposal to NSF in this area is being developed.

2. Characterization of pesticide spray solutions in agriculture, and polymer solutions and melts in manufacturing

The work in this area was guided by the needs and interests of researchers with the USDA in Wooster, Ohio, with whom I am collaborating. To address overspray of agricultural pesticides (due to spray drift and drop rebound from leaf surfaces) leading to groundwater contamination, the USDA needs to measure the rapid (on a sub millisecond timescale) decay of surface tension with surface age. Since surface tension controls droplet formation and drop rebound, regulations are based on this material property. With the USDA researchers we previously, in work described in a 1995 JFM paper, combined an inverse formulation of our model for an oscillating free surface jet with elliptical cross-section with free surface measurements of USDA experiments to quantify the decay of surface tension.

Experimental Results

Our progress in this area was driven by significant advances on the experimental front. Due to development of the apparatus and lighting, and improvements in data processing, we can now measure with high resolution *in two perpendicular views* the free surface profile, *slope, and curvature.* The two views allow us to apply the high-resolution modeling of oscillating jets, and the accurate measurement of slope and curvature has led to a powerful and exciting Method 2 in the inverse modeling, described below.

Modeling and the inverse problem

The analysis in the 1995 JFM paper considers the surface tension and viscosity constant within a wavelength of the oscillating jet free surface, which in the inverse formulation yields resolution of surface tension only on the order of 2 ms, during which surface tension can change 20%. I co-authored [6] with three USDA researchers, which utilized this analysis and free-surface measurements on USDA apparatus to characterize the rapidly changing surface tensions of a battery of pesticide solutions.

In [8], our previous equations for oscillating jets are extended to allow for surface tension to vary in space and time within the wavelength, and the new models are used to investigate the effect of decaying surface tension on oscillating jet behavior. This modeling advance, combined with the experimental advances described above, pushes our resolution of dynamic surface tension to fractions of a millisecond. An important result in [2] is the following: The rate and form of the decay can be inferred from downstream measurements, avoiding the need for measurements near the nozzle where rapid surface tension decay takes place. In [12] the equations for oscillating jets are extended to allow for shear-rate dependent viscosity. This modeling advance allows us to employ for the first time the oscillating jet technique to characterize the non-Newtonian viscosity of pesticide solutions in rapidly oscillating, high strain-rate elongational flows. The results of [12] also have fundamental ramifications in non-Newtonian rheology.

In addition to working with the USDA to analyze oscillating jet measurements performed at their laboratory, in 1996 I began a collaboration with Kurt Koelling of the Department of Chemical Engineering at Ohio State to develop our own laboratory for high-resolution free surface measurements. This collaboration is advancing the USDA research, and is also addressing needs in the polymer processing industry. The first results, published in [4], combined measurements of axisymetric polymer solution filaments with our viscoelastic models to deduce extensional viscosities, relaxation times, and retardation times.

I have developed two ways to characterize the fluid using our spinline measurements, and have applied both of them in the oscillating jet application with the USDA and the polymer rheology effort:

Method 1

The measured upstream radius and slope are used as initial conditions, and the solution to the forward problem is computed for trial values of material properties; the computed free surface profile is then compared with the measured profile and the material properties are adjusted to produce a better match, iterating to a best fit. This trial-and-error strategy is the standard approach to the inverse problem for material characterization. Its advantage is that it demands only an accurate measurement of the profile; slope is required only at $z = 0$ and the curvature is not required. The disadvantages are (i) the method will only give the best values of material constants within a specific assumed form of the constitutive function, and can give no guidance as to the correct form (e.g. it cannot tell if the fluid is rate-dependent or viscoelastic), and (ii) with the many-dimensional, nonlinear equations of the forward problem, it is in general impossible to devise an automated convergent iteration scheme.

Method 2

This method is new and powerful. It is only possible because of our recent ability to measure with high resolution the spinline kinematics through three orders (profile, slope, curvature). With these measurements all of the kinematical quantities and their derivatives that appear in the momentum and constitutive equations are known functions (the kinematics appear through curvature in these equations), in which case the momentum and constitutive equations decouple: the momentum equations with known kinematics dictate what evolution of stress must be present in the spinline to balance inertia, gravity, and surface tension, and the constitutive equations dictate what stress is generated by those kinematics. The stress generated by momentum considerations must be correct, hence we adjust *the form of the constitutive equation and constants in the form* to get a *pointwise* match of the two stresses. We are also in the process of adapting this method to directly deduce the form and rate of decay of surface tension.

3. Criteria for Admissible Forms of Non-Newtonian Viscosity for Flows with Low Strain Rates

The observations in [12] have an important ramification in non-Newtonian constitutive modeling. It is well understood that use of the power law form for viscosity should be avoided with shear thinning fluids in flows with low strain rates, due to the unbounded viscosity at zero shear rate predicted by this model. This caution is borne out in the oscillating jet flow (which oscillates through zero shear rate) not in the leading order solution, but instead in unbounded spikes in the next-order correction at every location of zero strain rate. An important question for a shear thinning fluid is how to specify viscosity as a function of strain rate in such a way that it is physically realistic at zero and low strain rates. In [13] we investigate three modifications of the power law form which are expressly designed to remedy problems at low strain rates, by assigning finite zero strain rate viscosities. We find that this in itself does not remove the spikes and therefore the problem of an invalid asymptotic expansion at zero strain rate in the oscillating jet solution. In a physical experiment, the fluid to be modeled is observed to undergo the slowly varying steady oscillating jet flow, without the occurance of small length scales and subsequent jet breakup; when modeling the oscillating jet flow, an acceptable non-Newtonian constitutive form must yield a solution which is similarly stable. The proposed viscosity as a function of strain rate must therefore possess, in addition to a bounded zero strain rate viscosity, a sufficiently small gradient at zero strain rate. Intuitively, one might suspect that to be admissible the viscosity should be effectively Newtonian at low strain rates, i.e. zero viscosity gradient at zero strain rate; we find that the gradient need not be zero, but just not be too large. This requirement on the viscosity form transfers to any application in which the flow experiences zero or low strain rates.

4. Modeling of industrial filament manufacturing processes

I am continuing to bring to publication the knowledge gained through modeling of HCC processes. Four papers have appeared in this area [3, 5, 7, 17], one paper and a book chapter are in press [9, 16], and two papers are near submission [14, 15]. Another paper, "The Interaction and Cooling of Multiple Fibers in Melt-Spinning Processes," is in preparation.

5. Modeling of fiber drawing and belt power transmission

One of the problems motivated by my interaction with HCC is the modeling of the fiber drawing stage of the filament manufacturing process after melt spinning. In this steady-state process the solidified filament is stretched by a factor of on the order of 100% as it proceeds along a path that wraps around a series of pairs of large diameter rollers, each rotating at speeds faster than the one before. It turns out that the filament stretching happens not in the free spans between rollers, but on the roller surfaces. Our literature search revealed that there has been no modeling of the stretching of a filament on a roller, so we have produced such a model [11].

We found that our model removes a gap in another field, far removed from polymer processing: In the problem of power transmission between two axles using a belt and pulleys, handbooks typically employ equations based on a static belt on static pulleys, even though in the actual situation belts and pulleys are moving, often at high speeds. To remedy this error, some studies include a correction for centrifugal acceleration. No one, however, accounts for the acceleration of the belt due to stretching, an effect captured in our fiber drawing model. We have found that the stretching effect meaningfully modifies important predictions such as the zones of slip between belt and pulley, and the maximum torque and power that can be transmitted by the system.

6. High strain-rate plasticity

Our analytical and experimental tools we developed to attack problems in fluid mechanics and rheology of liquid fiber flows have directly led (helped by a fortuitous collaboration with Glenn Daehn in the Department of Material Science and Engineering at Ohio State) to advances in an active area in solid mechanics and material science, high strain-rate characterization. To design manufacturing processes in which high strain rates occur there is a need to characterize the material. High strain-rate characterization is also important for crashworthiness, machining operations, high velocity impact, and fracture. The work described here is in [10]; a proposal to ARO is also being developed. We exploit an experiment (performed in Prof. Daehn's lab) in which a specimen ring is placed over a solenoid and, when a large capacitor is discharged into the solenoid, is given via direct magnetic induction an impulsive load in an radially outward direction. Our modeling expertise translates to this slender ring problem, enabling us to derive equations which relate using Maxwell's equations and momentum considerations the rapidly changing hoop stress in the ring to the expanding ring radius and solenoid and ring currents. Our advances in the inverse modeling also transfer: in [4] we apply our model for high strain-rate material characterization in the two ways described earlier: 10

The expanding ring radial velocity is experimentally known from a Velocity Interferometer System for Any Reflector (VISAR). In Method 1 a form of the constituitive equation for the material is proposed, and the values of coefficients are varied until the ring radial velocity as a function of time predicted by the forward problem best fits the measured ring expansion. In Method 2 the ring velocity measured with the VISAR is numerically integrated and differentiated to yield strain ε, rate of strain $\dot{\varepsilon}$, rate of rate of strain $\ddot{\varepsilon}$, etc. The ring velocity is also inserted into the combined Maxwell's equation/momentum equation to infer the ring stress $T_{\theta\theta}$. The combination of this information is the path in $(T_{\theta\theta}, \varepsilon, \dot{\varepsilon}, \ddot{\varepsilon})$ space for the experiment. The paths of many experiments will reveal the surface in $(T_{\theta\theta}, \varepsilon, \dot{\varepsilon}, \ddot{\varepsilon})$ space that characterizes the material. Again, we feel that this second method is more powerful, as it not only returns values of material constants, but also reveals the form of the contitutive function. For instance, if the material has no strain-rate dependence, paths for all experiments at the same value of strain will intersect at the same value of stress, even though the experiments have differing strain rates.

7. Foam generation and flow

I am directing the dissertation research of a Ph.D. student who is employed by General Electric at their refrigerator manufacturing plant in Louisville (and supported in his studies by GE). Together we are modeling the GE problem of the generation and flow of a foam to fill the hollow cavities of the refrigerator walls to become when it hardens the solid foam insulation. The current task is to characterize the flow properties of the reactive foam; the next will be to model the cavity filling and solidification. The problem is similar to my experience of modeling manufacturing processes at HCC. It is hoped that a similar situation will develop with GE, in which GE becomes a source of challenging and industrially relevant problems, and our academic knowledge can be transfered to address their needs.

Joint Air Force Research Laboratory/DAGSI Proposals

Professor Anthony Palazotto of the Department of Aeronautics and Astronautics at the Air Force Institute of Technology in Dayton heard about my modeling of industrial processes and contacted me. I faxed him a copy of the research summary I prepared for you in August, and drove to AFIT 7 November 1998 to visit him and William Baker, Associate Professor of Mathematics.

As an outgrowth of that meeting I collaborated with Prof. Palazotto in two AFRL/DAGSI proposals, in response to topics generated by the Air Vehicle Directorate of WPAFB:

1. Advanced Shielding Concepts for Space Systems

This proposal was in response to Arnold Mayer's requests in the area of Nonclassical Materials, Structures, Thermal Energy Management and Stability of Aircraft Subsystems: "We seek to understand momentum/energy interactions and extent of the damage and its morphology inflicted by ballistic projectiles and nearby and internal explosions on aircraft structure and containing walls of compartments or fuel tanks built of fiber-reinforced polymer-matrix composites that is immersed in a high-speed airstream. In connection with the development of survivability concepts which allow damage but avoid catastrophic distruction, ability to analyze and predict the simultaneous evolution of deformation and damage of a structure subjected to an impulsive load (impact or explosion) is desired."

This project demands the characterization of the high strain-rate response of the fiber-reinforced polymer-matrix composites. Prof. Palazotto feels that the novel characterization technique I am developing (described in item 6 above) will have important advantages over existing techniques for characterization of high strain-rate plasticity. This effort also addresses the closely allied needs of Jeffrey Calcaterra relating to developing new material systems, structural concepts, and analytical methods for shielding on next generation space systems, particularly the Space Operations Vehicle (SOV).

This proposal passed the first cut down to forty, of which ten will be funded.

2. Nonlinear Dynamic Behavior in Smart Composite Curved Panels

This proposal did not make the first cut. It was in response to the request of Narendra Khot: "The objective of this research is to investigate nonlinear dynamic stability of curved panels applicable to air vehicle structures. The topic will include:

1) Chaotic behavior of composite shell structures.

2) Development of efficient numerical techniques for evaluating material response due to large strains brought about by large displacements and rotations.

3)Formulation and development of active control systems to supress large displacements to prevent instability."

Prof. Palazotto felt that the coupling of the momentum and electromagnetic equations employed in the research modeling electromagnetic ring expansion of item 6 above also could apply directly to this effort, in the formulation and development of active control systems. In addition, he was confident that the abilities and program of attack that led to my success in modeling fiber spinning and agricultural processes with nonlinear dynamic equations and analyzing these equations would succeed in this application.

Publications acknowledging funding from F49620-97-0003

Refereed Journal Publications

1. S.E. Bechtel, D. Cao, and H. Hsiao, "Geometry and Heat Loss in Channel Flow of a Fluid with Temperature-Dependent Density," AIChE Journal, v. 42, n. 9, September 1996, pp. 2453-2466.

2. D. Cao, S.E. Bechtel, and M.G. Forest, "Thermomechanical Equations Governing a Material with Prescribed Temperature-Dependent Density, with Application to Nonisothermal Plane Poiseuille Flow," ASME J. of Applied Mechanics, v. 63, n. 4, December 1996, pp. 1011-1018.

3. Q. Wang, M.G. Forest, and S.E. Bechtel, "1-D Models for Thin Filaments of Liquid Crystalline Polymers: Coupling of orientation and Flow in the Stability of Simple Solutions," Physica D, v. 99, n. 4, 1997, pp. 527-554.

4. V.V. Ramanan, S.E. Bechtel, V. Gauri, K.W. Koelling, and M.G. Forest, "Exploiting Accurate Free Surface Jet Measurements for Material Characterization," J. of Rheology, v. 41, n. 2, March/April 1997, pp. 283-306.

5. Q. Wang, M.G. Forest, and S.E. Bechtel, "1-D Isothermal Spinning Models for Liquid Crystalline Polymer Fibers," J. of Rheology, v. 41, n. 4, July/August 1997, pp. 821-850.

6. D.L. Reichard, J.A. Cooper, S.E. Bechtel, and R.D. Fox, "A System for Determining Dynamic Surface Tension Using the Oscillating Jet Technique," Atomization and Sprays, v. 7, 1997, pp. 219-233.

7. G.M. Henson, D. Cao, S.E. Bechtel, and M.G. Forest, "A Thin-Filament Melt Spinning Model with Radial Resolution Stress," J. of Rheology, v. 42, n. 2, March/April 1998, pp. 329-360.

8. S.E. Bechtel, M.G. Forest, N. Youssef, and H. Zhou, "The Effect of Dynamic Surface Tension on the Oscillation of Slender Elliptical Newtonian Jets," ASME J. of Applied Mechanics, v. 65, n. 3, September 1998, pp. 694-704.

9. S. Naboulsi and S.E. Bechtel, "Bicomponent Newtonian Filaments," Physics of Fluids, to appear April 1999.

10. W. Pon, G.M. Henson, S.E. Bechtel, G.S. Daehn, and M.G. Forest, "A Model for Axisymmetric High Strain-Rate Electromagnetic Ring Expansion, and its Application to Material Characterization," submitted to J. of Applied Physics.

11. S.E. Bechtel, S. Vohra, K.I. Jacob, and C.D. Carlson "The Stretching and Slipping of Belts and Fibers on Pulleys," submitted to J. of Applied Mechanics.

12. N. Youssef, S.E. Bechtel, M.G. Forest, H. Zhou, and K.W. Koelling, "Non-Newtonian Oscillating Elliptical Free Surface Jets, and Criteria for Admissible Forms of Non-Newtonian Viscosity for Flows with Low Strain Rates," to be submitted to ASME J. of Applied Mechanics.

13. F.J. Rooney, S.E. Bechtel, Q. Wang, and M.G. Forest, "Modeling of Thermal Expansion: Instabilities of Constrained Theories and Constitutive Limits," to be submitted to J. of Fluid Mechanics.

14. G.M. Henson and S.E. Bechtel, "Radially Dependent Stress and Modeling of Solidification in Melt Spinning," to be submitted to International Polymer Processing.

15. H. Hsiao, D. Cao, S.E. Bechtel, and M.G. Forest, "Nonisothermal Fiber Spinning with Temperature-Dependent Stress," to be submitted to J. of Polymer Science.

Book Chapter

16. S.E. Bechtel, M.G. Forest, Q. Wang, and H. Zhou, "Free Surface Viscoelastic and Liquid Crystalline Polymer Fibers and Jets," in *Advances in the Flow and Rheology of Non-Newtonian Fluids*, D.A. Siginer, D. DeKee, and R.P. Chhabra, editors, Elsevier Science, Rheology Series, in press.

Refereed Proceedings Article

17. S.E. Bechtel, J.G. Cao, and M.G. Forest, "Viscoelastic Free Surface Jets and Filaments," in *Rheology and Fluid Mechanics of Nonlinear Materials*, S.G. Advani and D.A. Siginer, editors, FED-Volume 243, MD -Volume 78, ASME Press, New York, 1997, pp. 21-32.

Presentations

Invited Talks

"Viscoelastic Free Surface Jets and Filaments," Symposium on Rheology and Fluid Mechanics of Nonlinear Materials," ASME International Mechanical Engineering Congress and Exposition, Dallas, Texas, November 1997.

"Modeling of Polymer Manufacturing Processes," Mechanical Engineering Seminars, The Ohio State University, Columbus, Ohio, January 1998.

"Modeling of the Manufacturing of Polyester Fibers," School of Textile and Fiber Engineering Seminar, Georgia Institute of Technology, Atlanta, Georgia, April 1998.

"Thermomechanics and Stability of Materials with Temperature-Dependent Density," Applied Mathematics Seminar, University of North Carolina, Chapel Hill, North Carolina, September 1998.

Contributed Presentations

"Material Characterization in Extensional Flows Using the Fiber-Spinning Process," Symposium on Rheology and Fluid Mechanics of Nonlinear Materials," XIIth International Congress on Rhology, Quebec City, Canada, August 1996.

"Radial Resolution of Temperature and Stress in the Melt Spinning of Fibers," Fiber and Film Processing Symposium, 1996 AIChe Annual Meeting, Chicago, Illinois, November 1996.

"Exploiting Accurate Free Surface Jet Measurements for Material Characterization," Fiber and Film Processing Symposium, 1996 AIChe Annual Meeting, Chicago, Illinois, November 1996.

"A Thin-Filament Melt Spinning Model with Radial Resolution Stress," Symposium on Rheology and Fluid Mechanics of Nonlinear Materials," 69th Annual Meeting of the Society of Rhology, Columbus, Ohio, Oct. 1997.

"A Constrained Theory for Materials with Prescribed Temperature-Dependent Density," 13th U.S. National Congress of Applied Mechanics, Gainesville, Florida, June 1998.