Research on

POLYMER FLUID DYNAMICS:

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FLUID DYNAMICS IS A very old subject. The Navier-Stokes equations are about 150 years old, and libraries have shelves of books devoted to boundary-layer theory, turbulence, flow through porous media, gas dynamics, and other facets of this broad and useful discipline. Chemical engineers share with other engineers their interest in the applications of fluid dynamics and their responsibility for the further development of the basic science of fluid dynamics.

There are several subfields of fluid dynamics in which chemical engineers have particularly strong responsibilities: fluid dynamics of reactive systems, fluid dynamics of diffusing systems, two-phase and multiphase flow systems, and polymer fluid dynamics. The flow of polymer solutions and polymer melts quite properly belong in the domain of chemical engineering for several reasons:

- **Chemical engineers are normally charged with the development of design procedures involving the "unit operations" of the polymer industry: extrusion, blow molding, fiber spinning, etc.**
- **Chemical engineers have the background in organic chemistry needed for understanding polymer synthesis, solvent effects, chemical degradation, and molecular weight distributions.**
- **Chemical engineers have sufficient training in physical chemistry to understand optical phenomena, polymer kinetic theory, surface tension, polyelectrolytes, and phase equilibria.**
- **Chemical engineers have sufficient background in transport phenomena to tackle problems in non-Newtonian flow, viscous heating effects, mixing phenomena, and thermal dependence of transport properties.**

It is no wonder then that chemical engineers have in the past several decades developed strong research programs and new courses in polymer fluid dynamics. In so doing the chemical engineering professor has had to build strong bridges to adjacent disciplines, particularly continuum mechanics, polymer chemistry, and applied mathematics. Chemical engineers are currently involved in at least ten kinds of problems in polymer fluid dynamics, and in the following summary we try to indicate what the objectives and challenges are:

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Development of Constitutive Equations. It is well known that polymeric liquids do not obey Newton's law of viscosity; many simple experiments show this conclusively [1]. The stress tensor (at the present time t) for fluids made up of small molecules is given simply in terms of the velocity gradients at the time t. For polymeric fluids, however, the stresses in a fluid element at the present time t depend in a complicated way on the velocity gradients experienced by that fluid element over all past times t′; that is, "memory effects" are involved. One of the central problems of the field is to obtain expressions for the stress tensor (the "constitutive equation" or the "rheological equation of state"). This problem is still only partially resolved. We have fragmentary answers provided by rheometric experiments, by continuum mechanics, and by molecular theory.

Rheometry. One cannot go into the laboratory and "measure the stress tensor" in an arbitrary flow system. The best we can do is to measure some of the stress tensor components in very carefully controlled flow fields; this science of measurement is now called "rheometry" [2, 3]. There still remains much to be done in developing reliable instrumentation that can be used to measure viscosity, stress relaxation, elongational viscosity, complex viscosity, and a dozen or so other rheological properties. At the present we do not have nearly enough trustworthy rheometric data on carefully characterized samples (i.e., samples of known molecular weight, concentration, and molecular structure) to test the proposed constitutive equations and molecular theories.

Kinetic Theory. If one is given the molecular weight, concentration, and polymer structure, there are no formulas that one can turn to to predict with confidence the rheological properties that one needs for doing analysis or design of polymer flow systems or processing units. The past several decades have produced many new kinetic theories for polymeric liquids [4] and these have been very helpful in suggesting useful forms for constitutive equations. Work along these lines is continuing, both for dilute solutions [5] and for polymer melts; for the latter, there are now two very different kinds of competing theories, the "network theories" [6, 7] and the "reptation theories" [8, 9]. A number of investigators are also approaching the structure-rheology relationship through the use of computer simulation techniques, but this method is in its infancy.

Solution of Flow Problems. Once one has settled on a reasonable constitutive equation (and there is at this moment still a great deal of subjective judgment as to what "reasonable" is) then one is faced with another enormous challenge, namely that of solving the equations of continuity and motion along with the constitutive equation in order to predict velocity profiles. There are a few trivial flows where one can get some analytical solutions, or possibly even solutions by use of perturbation theory [10]. But most problems of interest to the engineer necessarily require numerical analysis. Such numerical problem-solving taxes even the biggest computers because of the necessity of taking into account the memory effects. Current efforts seem to have met only with moderate success; apparently computer solutions break down when the Deborah number (ratio of the time constant of the fluid to the characteristic time of the flow) becomes equal to about unity—and this is just the beginning of the exciting region where the "elastic effects" begin to be important [11].

Flow Visualization. Because of the problems just mentioned it is of particular importance that polymer fluid dynamicists develop techniques for flow visualization and for the complete measurement of velocity fields (e.g., by using laser-doppler methods) in a variety of flow systems [12, 13]. We need to know much more about the various "flow regimes," particularly the conditions where various kinds of instabilities occur. It is important, too, that the fluids used in these flow visualization experiments be characterized rheometrically; that is, it is essential to know the non-Newtonian viscosity curves, the normal stress curves, and other material functions in order to be able to interpret the flow experiments. In many industrial problems, flow visualization is particularly important. Very little progress can be made in theorizing until the basic experimental facts are known.

Heat Transfer Studies. Because of the very high viscosities of concentrated polymer solutions and melts, the viscous energy dissipation is, more often than not, non-negligible. Most high-speed extrusion processes, injection molding systems, and other industrial operations involve appreciable viscous heating [14] and highly non-isothermal conditions. As a result it is necessary to put temperature dependence into the constitutive relations [15] and to study the rheological material functions as a function of temperature.

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Flows with Phase Change. Not only does one have to study nonisothermal problems, but also problems in which solid-liquid or liquid-solid transitions are occurring. In extruder operation one has to melt the polymer pellets upstream from the extrusion device. In all plastics manufacturing processes, one has to cool the molten polymer to obtain the finished product. In some instances the cooling and solidification occurs when the polymer is still in motion. Such problems involve both the kinetics of phase change, crystallization, heat transfer, and two-phase flow [16].

Two-Phase Flow. The widespread use of various kinds of fillers in the fabrication of composites brings up the subject of two-phase flow: solids, liquids, or gases dispersed in a fluid which is viscoelastic. Some of the most challenging problems facing the polymer fluid dynamicist in the polymer industry are those pertaining to the break-up of particle aggregates, mixing and blending, particle orientation in flow fields, distortion of gas bubbles, interfacial phenomena, and alteration of mechanical and optical properties of the melt and the solid finished product. Not nearly enough is known about the clustering of particles and the distribution of particles in concentrated two-phase systems [17].

Polymer Unit Operations. All of the topics listed above can be important in the development of a better understanding of the polymer unit operations. It is not enough, however, to analyze existing processes and equipment. The chemical engineer must also be concerned with improving the equipment design and the process operation. In addition, he has the even more challenging task of trying to develop totally new fabrication methods [16], often collaborating with mechanical and electrical engineers. Most of this kind of inventive work has been done in industry, where personnel and equipment resources are more plentiful than in the university. However, cooperative projects or consulting activities can be very important in bridging the gap between the academic fluid mechanicist and the industrial designer.

Drag Reduction. There are several phenomena pertaining specifically to dilute solutions that have been the subject of intensive research. The oldest and most important of these is "drag reduction" [18]. The addition of small amounts of a polymer to a Newtonian liquid can reduce significantly the friction factor in turbulent flow. The understanding of this phenomenon presents an enormous challenge, since it combines two very difficult fields: turbulence, and viscoelasticity. Perhaps some of the recent advances in the kinetic theory of dilute solutions will be used to elucidate this fascinating phenomenon.

IT SHOULD BE EVIDENT from the above listing of problem areas that the field of polymer fluid dynamics is enormous in extent and variety. All of the above topics are interrelated, and the study of any one part of the field invariably leads to some other part of the subject. In polymer fluid dynamics one can seek all kinds of challenges: mathematical, physical, chemical, process design, equipment design, computing, and instrumentation. □

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REFERENCES

1. R. B. Bird, R. C. Armstrong, and O. Hassager, "Dynamics of Polymeric Liquids, Vol. 1: Fluid Mechanics," Wiley, New York (1977) — Ch. 3.
2. K. Walters, "Rheometry," Chapman and Hall, London (1975).
3. R. W. Whorlow, "Rheological Techniques," Wiley, New York (1980).
4. R. B. Bird, O. Hassager, R. C. Armstrong, and C. F. Curtiss, "Dynamics of Polymeric Liquids, Vol. 2: Kinetic Theory," Wiley, New York (1977).
5. R. B. Bird, P. J. Dotson, and N. L. Johnson, J. Non-Newtonian Fluid Mech., *7*, 213-235 (1980).
6. A. S. Lodge, Rheol. Acta, *7*, 379-392 (1968).
7. M. H. Wagner, Rheol. Acta, *18*, 33-50 (1979).
8. M. Doi and S. F. Edwards, J. Chem. Soc., Faraday Trans., II, *74*, 1789-1832 (1978); *75*, 38-54 (1979).
9. C. F. Curtiss and R. B. Bird, "A Kinetic Theory for Polymer Melts," U. Wisc. Theo. Chem. Inst. Reports 636 and 637, May, 1980.
10. R. B. Bird, R. C. Armstrong, and O. Hassager, op. cit., Chs. 5 through 9.
11. R. C. Armstrong, personal communication.
12. M. Gottlieb and R. B. Bird, Ind. Eng. Chem. Fund., *18*, 357-368 (1979).
13. R. L. Christiansen, Ph.D. Thesis, U. Wisconsin (1980).
14. H. H. Winter, Adv. Heat Transfer, *13*, 205-267 (1977).
15. G. Marrucci, Trans. Soc. Rheol., *16*, 321-330 (1972).
16. Z. Tadmor and C. G. Gogos, "Principles of Polymer Processing," Wiley, N.Y. (1979).
17. A. L. Graham, PhD Thesis, U. Wisconsin (1980).
18. H. S. Stephens and J. A. Clarke, eds., "Proc. Second International Conference on Drag Reduction at Cambridge," BHRA Fluid Engineering, Cranfield (1977).