COMPUTATIONAL RHEOLOGY WITH INTEGRAL CONSTITUTIVE EQUATIONS

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Abstract

Computational rheology deals with the formulation and solution of constitutive equations for non-Newtonian materials. From these the emphasis is put on polymeric materials, which exhibit both viscous and elastic behaviour in flow and deformation. These materials are often called viscoelastic materials. Polymer solutions and melts (*e.g.* commercial plastics and rubber) are good examples of viscoelastic materials. Their processing under continuous (*e.g.* extrusion) or batch (*e.g.* injection molding) operations is the main occupation of the plastics and rubber industries, but the corresponding modelling and numerical simulation is a difficult task and a relatively recent undertaking.

The present work reviews modelling aspects of viscoelasticity and shows how the complex rheology of these materials is best captured through integral constitutive equations with a spectrum of relaxation times. Using such constitutive equations and the Finite Element Method (FEM), the solution of some benchmark problems of rheology becomes feasible. Examples will be shown from the flow of polymer melts and solutions in a 4:1 axisymmetric contraction encountered in standard capillary rheometry, as well as the flow around a sphere falling in a cylindrical tube. The emphasis will be on demonstrating the flow patterns via streamlines and predicting such viscoelastic phenomena as vortex growth, extrudate swell, and reduction of the drag coefficient, which are of particular interest to the rheological community as test cases of computational results.

Zusammenfassung

Die computergestützte Rheologie beschäftigt sich mit der Formulierung und der Lösung rheologischer Zustandsgleichungen nichtlinearer Stoffe. Ausgehend davon stehen im Mittelpunkt Polymere, die sowohl viskoses als auch elastisches Verhalten in der Strömung und bei Deformationen aufweisen. Diese Materialien werden häufig als viskoelastische Stoffe bezeichnet. Polymerlösungen und -schmelzen (kommerzielle Kunststoffe und Gummis) sind gute Beispiele für viskoelastische Stoffe. Ihre Verarbeitung in kontinuierlichen Prozessen (z.B. Extrusion) oder in Stückprozessen (z.B. Spritzgießen) stellt die Hauptanwendung in der Kunststoff- und der Gummiindustrie dar. Die entsprechende Modellierung und numerische Simulation sind jedoch eine komplizierte Aufgabe und ein vergleichsweise neues Gebiet.

Die vorliegende Arbeit stellt die wesentlichen Gesichtspunkte der Modellierung der Viskoelastizität zusammen und zeigt, wie die komplexe Rheologie dieser Stoffe am besten durch Zustandsgleichungen von integralem Typ mit einem Relaxationszeitspektrum berücksichtigt werden kann. Unter Zugrundelegung solcher Zustandsgleichungen und der Methode der finiten Elemente (FEM) wird die Lösung einiger ”Werkstatt-Probleme“ der Rheologie möglich. Exemplarisch wird die Strömung von Polymerschmelzen und -lösungen sowohl in einem 4:1 rotationssymmetrischen konischen Fließkanalübergang in Standard-Kapillarrheometersystemen als auch in einer Strömung um eine Kugel, die in ein Zylinder eintaucht wird, berechnet. Akzente bilden die Demonstration des Strömungsmusters und die Vorhersage viskoelastischer Phänomene wie Wirbelwachstum, Strangaufweitung und die Reduktion des Schleppkoeffizienten, die von spezieller Interesse der Rheologen als Testmethode für die Ergebnisse der Computerberechnungen sind.

Résumé

La rhéologie par ordinateur s'intéresse à la formulation et à la résolution d'équations constitutives pour les matériaux non newtoniens. Parmi ces matériaux, nous nous intéressons plus particulièrement aux matériaux polymères qui présentent un comportement à la fois visqueux et élastique quand ils sont soumis à un écoulement ou une déformation. Ces matériaux sont souvent appelés matériaux viscoélastiques. Les solutions de polymère et les fondus de polymère (par exemple les plastiques commerciaux et les caoutchoucs) sont de bons exemples de matériaux viscoélastiques. Leur mise en oeuvre par des opérations en continue (par exemple l'extrusion) ou en lots (par exemple le moulage par injection) est la principale préoccupation des industries de plastiques et caoutchoucs. Mais la modélisation et la simulation numérique de la mise en oeuvre sont une tâche difficile et ont été entreprises assez récemment.

Cet article est une revue de la modélisation de la viscoélasticité et montre comment la rhéologie complexe de ces matériaux est mieux décrite par des équations constitutives integrales avec un spectre de temps de relaxation. En utilisant de telles équations constitutives et la méthode d'élément fini (FEM), la résolution de problemes cruciaux de rhéologie devient possible. Des exemples seront présentes: l'ecoulement de solutions et fondus de polymére dans une contraction axisymetrique de type 4:1 recontrée en rhéometrie capillaire classique et l'écoulement autour d'une sphére tombant dans un tube cylindrique. L'accent sera mis sur l'imagerie de l'écoulement au moyen de lignes de courant et sur la prédiction de phénomènes tels que la croissance de vortex, le gonflement d'un extrudé, la reduction du coefficient d'étirement, qui sont d'un interet particulier pour la communauté des rhéologues, puisque ce sont des cas types pour tester les rèsultats des simulations.

Key-words:
Computational rheology, integral constitutive equations, viscoelasticity

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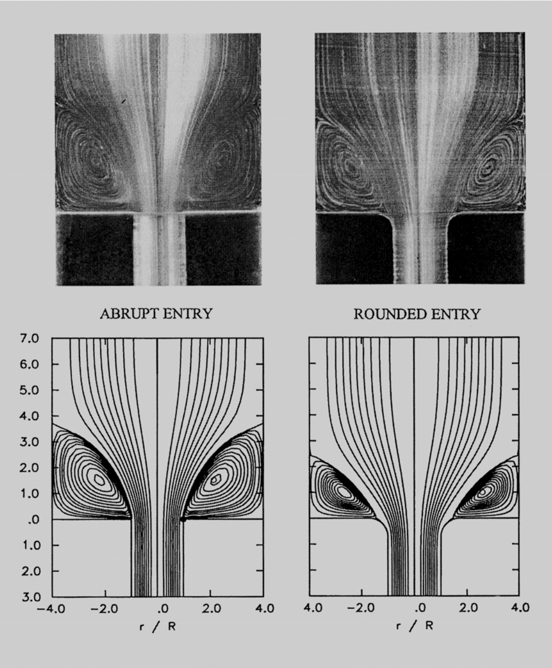

Figure 4 (left): Streamline patterns at Ws = 4 (see Eq. 7) for the flow of the S1 test fluid (polymer solution PIB/PB) at 21°C through a 4:1 axisymmetric contraction: (upper half) experiments [16], (lower half) simulations [17].

The K-BKZ model with the PSM strain-memory function and the Luo-Tanner modification has been used, first to rheologically characterize the material (a standard IUPAC low-density polyethylene melt, LDPE-Melt A at 150°C). The results have been given in Figures 1 and 2 and Table 1. Then, numerical flow simulations have been undertaken by increasing the flow rate. The results are shown in Figure 3, as streamline patterns [13]. It is interesting to note the dramatic increase in vortex growth and extrudate swelling after the orifice, as the melt is extruded in the atmosphere. Swell ratios of up to 3 are obtained. These results are in very good agreement with the experimental data collected from a worldwide effort by Meissner [12].

For the case of a polymer solution, the rheological community has come up with an elastic liquid, which is a shear-thinning test fluid of polyisobutylene in polybutene (PIB/PB), nicknamed S1 fluid. Proper rheological characterization has been performed, and the data have been fitted with the K-BKZ model with 4 relaxation modes [16]. The corresponding numerical simulations have been performed in a recent study [17] and show a good correspondence between theory and experiments, as evidenced in Fig. 4, for the highest experimental flow rates.

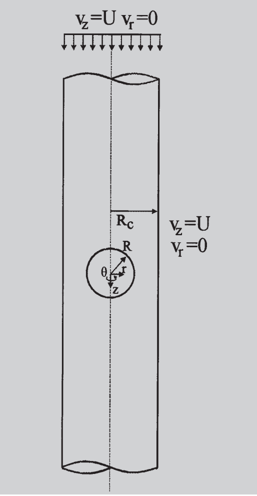

Figure 5: Domain definition and boundary conditions for the benchmark problem of falling sphere in a tube.

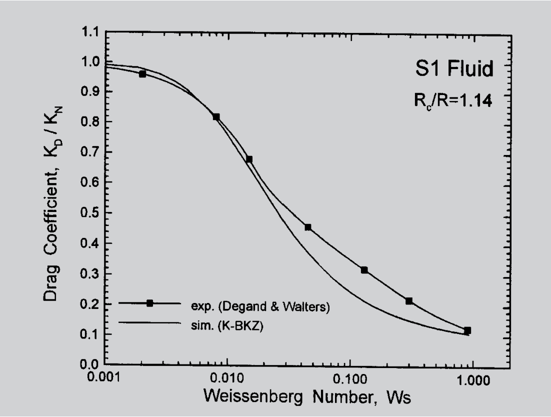

Figure 6: Drag coefficient vs. Weissenberg number for the shear-thinning test fluid S1 [19]. Symbols are experimental data reported by Degand and Walters [18].

5.2 EXAMPLE 2: FLOW AROUND A SPHERE – DRAG COEFFICIENT RESULTS

Another benchmark problem in computational rheology has been assigned to the flow around a sphere falling inside a cylindrical tube. Figure 5 shows a schematic representation of the domain along with boundary conditions. Experiments have been conducted with the same S1 fluid as above by Degand and Walters [18] for a tightly fitting arrangement, where the cylinder to sphere diameter ratio is $R_c/R=1.14$. The drag coefficient is defined as

$$\frac{K_D}{K_N} = \frac{F}{6\pi\eta_o UR} \tag{9}$$

where F is the drag force exerted by the fluid on the sphere, and K_N is the Stokes drag coefficient for a corresponding Newtonian fluid with a viscosity of η_o. Figure 6 shows the drag coefficient as a function of the Weissenberg number both for the experiments and the simulations, where a good agreement is obtained for the whole range of experimental observations. More on the subject can be found in [19].

6 CONCLUSIONS

Computational rheology has made good progress in recent years in the numerical simulation of viscoelastic materials. The use of multimode models, such as the integral K-BKZ model with a spectrum of relaxation times, has shown promise in reproducing experimental results in some special cases of rheology and rheometry. These include simple two-dimensional geometries, such as flow around a cylinder or a sphere, flow through contractions and extrusion dies.

Many unresolved problems still exist: they include among others, the incorporation of proper slip boundary conditions [20], strong temperature effects [21], problems with complex free sur-

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faces [22], and of course, the full three-dimensional non-isothermal simulations, which are in the process of being performed by different groups around the world. With the increasing speed of computers available to researchers, as well as taking into account the concerted effort by many different groups around the world, these problems are bound to be solved and ultimately help the polymer processing industry to design more effectively equipment for better processing and products.

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BIOGRAPHY

Evan Mitsoulis was born in 1954 in Athens, Greece. He received a Diploma in Chemical Engineering from the National Technical University of Athens (NTUA) in 1977, an M.Sc.E. from UNB in 1979, and a PhD from McMaster University in 1984, all in Chem. Eng. In 1984 he joined the Department of Chemical Engineering at the University of Ottawa, Canada, as an Assistant Professor. Since 1994 he is Professor and Director of the Computer-Aided Materials Processing Rheology & Design (CAMP-R&D) lab and research group. In 1998 he joined NTUA as Professor of Mining Engineering and Metallurgy, where he currently teaches. His research interests include computational rheology, non-Newtonian fluid mechanics, polymer and materials processing.

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