HSR 2001

BOOK OF ABSTRACTS

3rd International Meeting of the Hellenic Society of Rheology

Dedicated to Professor Andreas Acrivos
on the occasion of his Retirement

June 10-14, 2001
Patras, Greece

Preface

The Hellenic Society of Rheology was officially formed on June 16th, 1996, in Athens, Greece. Thus came into fruition the original attempts by the late Professor Tasos Papanastasiou to organize the Greek Rheological community and the many scientists and engineers who practice rheology in their professional careers. The establishment of HSR was followed by its first meeting in Nicosia, Cyprus, July 4-5, 1996, where the first Executive was elected and the Constitution was ratified. That first meeting had been dedicated to the memory of Professor Tasos Papanastasiou (1953-1994) and was attended by about 50 scientists and engineers.

The second meeting of the Society took place in Heraklion, Crete, August 31-September 2, 1998, with the participation of more than 60 people. The second meeting established the Hellenic Society of Rheology as one of the most rapidly growing scientific societies in Greece. As a result of the efforts of all its members, HSR subsequently became a member of the *European Society of Rheology* and the *International Committee on Rheology.* Given the success of the first two Meetings, the Society decided that an international symposium be organized under its auspices once every three years, periodically among the cities of Nicosia, Heraklion, Patras and Athens.

As a result of this resolution, the third International Conference of the Hellenic Society of Rheology (HSR) takes place in Patras, Greece, June 10-14, 2001. It is co-organized by the Institute of Chemical Engineering and High-Temperature Chemical Processes (ICE/HT-FORTH), the University of Patras (Department of Chemical Engineering), and the National Technical University of Athens (Department of Mining and Metallurgical Engineering).

HSR is a small society, its membership currently being about 45 people. Despite its small size, it is its mission to organize National and International Meetings of the highest quality, which will provide a common meeting ground to a number of rheologists both in Greece and abroad. It is hoped that the third International Conference, and its high-quality scientific program with contributions by first-rate researchers from all over the world, serves the most towards the fulfillment of this mission.

The third International Conference of the HSR is a special one, since it is dedicated to Professor **Andreas Acrivos**, one of the most influential chemical engineers of the last 50 years, on the occasion of his retirement from the City College of the City University of New York, where he held the A. Einstein Chair at the Levich Institute. Professor Acrivos' research interests lie in the general areas of Applied Mathematics, Newtonian and non-Newtonian Fluid Mechanics, Transport Phenomena and, currently, in the rheology of concentrated suspensions and the study of the effective properties of two-phase materials. He has published more than 180 papers in well-reputed journals, and has graduated a large number of Ph.D. students who, in their majority, have become leading scientists and engineers. His academic tree includes more than 400 members. He has received a number of distinguished awards, which include election to the U.S. National Academy of Engineering, the U.S. National Academy of Sciences, and the U.S. Academy of Arts and Sciences.

In order to honor Professor Acrivos, HSR invited a number of his former students, academic descendents and associates whose career has been influenced by him, as well as a fair number of internationally recognized researchers to participate in the Conference. Almost all of them gladly accepted to participate in the Conference as invited lecturers.

This volume is a compilation of the Abstracts of the presentations given in the Conference. The program includes 25 invited lectures spread in 5 different sessions which are dedicated to Professor Acrivos, 1 plenary presentation by Professor Acrivos, 51 oral presentations and 13 poster presentations. They cover a broad range of topics encompassing all areas of the general theme of Rheology: Polymer melts and solutions, colloids and suspensions, molecular modeling and simulations, and experimental, theoretical, and computational fluid dynamics.

Extended versions of some of the papers presented in the Conference have been submitted for publication in a special issue of the *Journal of Non-Newtonian Fluid Mechanics (JNNFM),* which is expected to appear within the year. The Organizing and Scientific Committees of the Conference are grateful to Professor Ken Walters, editor of *JNNFM*, for providing this opportunity in honor of Professor Acrivos.

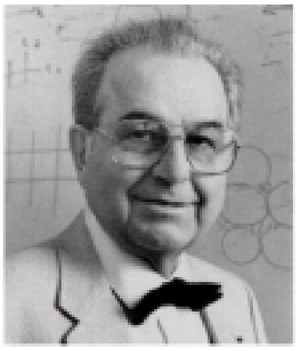
The organizers acknowledge the generous support of a number of universities, organizations and local companies, without the support of which this meeting would not have been possible. The tireless efforts of all the members of the Organizing and Scientific Committees and of the local organizing team, as well as of numerous individuals, are highly appreciated. To all of them, we would like to express our gratitude. We are particularly grateful to Kleanthi Zacharopoulou for her assistance throughout the many preparations for the Meeting and to Vasilis Bartzelas for his invaluable help with the preparation of the web page of the Meeting.

The organizers are extremely pleased to be your hosts in Patras for the duration of the Conference and wish you a pleasant stay and a productive Meeting.

Dr. Vlasis G. Mavrantzas
Chairman
Organizing Committee

Prof. John Tsamopoulos
Chairman
Scientific Committee

Patras, Greece
June 2001



ANDREAS ACRIVOS

Born in Athens, Greece, June 13, 1928

EINSTEIN PROFESSOR OF SCIENCE AND ENGINEERING
THE CITY COLLEGE OF THE CITY UNIVERSITY OF NEW YORK

Member: **National Academy of Engineering, USA**
National Academy of Sciences, USA
American Academy of Arts and Sciences, USA

A. Education

1. B.S., Syracuse University, 1950, Chemical Engineering
2. M.S., University of Minnesota, 1951, Chemical Engineering
3. Ph.D., University of Minnesota, 1954, Chemical Engineering

Dissertation: A Theoretical Discussion of Steady and Unsteady State Multicomponent Rectification including a Treatment of Mixtures with an Indefinite Number of Components
Research Director: Professor N.R. Amundson

B. Academic Experience

1. University of California, Berkeley, Department of Chemical Engineering
   Instructor, 1954-1955, Assistant Professor, 1955-1959, Associate Professor, 1959-1962

2. Stanford University, Department of Chemical Engineering
   Professor, 1962-1988, Professor Emeritus, 1988-present

3. The City College of the City University of New York
   Albert Einstein Professor of Science and Engineering, 1988-2001
   Professor Emeritus 2001-present

C. Current Research Interests

The rheology of concentrated suspensions; effective properties of two-phase materials; electrorheology

D. Organizations

1. American Chemical Society (Member)
2. American Institute of Chemical Engineers (Fellow)
3. American Physical Society (Fellow)
4. Society of Rheology (Member)
5. U.S. National Academy of Engineering (Member)
6. Editor of The Physics of Fluids, (1982-1998)
7. Member, U.S. National Committee on Theor. and Applied Mechanics (1980-2000), Chair (1984-1986)
8. Member of Congress Committee, IUTAM (1984-2000)
9. U.S. National Academy of Sciences (Member)
10. American Academy of Arts and Sciences (Fellow)
11. The New York Academy of Sciences (Fellow)

E. Honors and Awards

1. Humble Oil Lecturer, 1959
2. Guggenheim Fellow, 1959
3. PRF Unrestricted Research Award, Type C, 1962
4. A.P. Colburn Award, American Institute of Chemical Engineers, 1963
5. ASEE Lectureship Award, 1967
6. Professional Progress Award, American Institute of Chemical Engineers, 1968
7. William N. Lacey Lecturer, California Institute of Technology, 1972
8. Guggenheim Fellow, 1976
9. Elected to the U.S. National Academy of Engineering, 1977
10. Leon Lapidus Lecturer, Princeton University, 1980
11. Elected Fellow, American Institute of Chemical Engineers, 1980
12. Elected Fellow, American Physical Society, 1981
13. Sherman Fairchild Distinguished Scholar, California Institute of Technology, 1983-1984
14. W.K. Lewis Lecturer, Massachusetts Institute of Technology, 1984
15. Warren K. Lewis Award, American Institute of Chemical Engineers, 1984
16. G.I. Taylor Medal, Society of Engineering Science, 1988
17. Fluid Dynamics Prize, American Physical Society, 1991
18. Elected to the U.S. National Academy of Sciences, 1991
19. Julian C. Smith Lecturer, Cornell University, 1992
20. Berkeley Lecturer, University of California, 1993
21. Honorary Doctor of Science, Syracuse University, 1993
22. Elected Fellow of the American Academy of Arts and Sciences, 1993
23. Ascher Shapiro Lecturer, Massachusetts Institute of Technology, 1994
24. Bingham Medalist, Society of Rheology, 1994
25. Elected Fellow of the New York Academy of Sciences, 1994
26. Honorary Doctor of Science, Illinois Institute of Technology, 1995
27. L.S.G. Kovasznay Distinguished Lecturer, University of Houston, 1997
28. Honorary Doctor of Science, New Jersey Institute of Technology, 1998
29. Honorary Doctor of Science, University of Minnesota, 2000
30. Institute Lecturer, American Institute of Chemical Engineer, 2000

F. Publications

Professor A. Acrivos has authored and co-authored over 180 publications in International refereed Journals

G. Professional Influence

Many of his students and Associates hold Academic positions in world-known Academic Institutions. These are:

D.J. Wilde
J.D. Goddard
J.R. Bowen
J.C. Berg
Russ E. Davis
L.G. Leal
R. Robertson
Dominique Barthès-Biesel
Avi Nir
Arlindo de Almeida Rocha
W.B. Russel
A.S. Sangani
Francis A. Gadala Maria
John F. Brady
R.H. Davis
D. Leighton
Eric S.G. Shaqfeh
Ali Borhan

One of his numerous students in Industry is Andrew Grove, the current Chairman of the board of **Intel.**

His Academic Tree, which includes his students, their students and so on, has over **400 members!**

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E. Mitsoulis, Greece
S. Nychas, Greece
A. Payatakes, Greece
D. Theodorou, Greece
D. Vlassopoulos, Greece

HSR 2001 Program Summary

Monday, 11 June 2001
4 sessions dedicated to Prof. A. Acrivos

08:30-09:00	*registration*
09:00-09:30	*welcome remarks*
09:30-11:10	5 invited presentations
11:10-11:30	*coffee break*
11:30-12:50	4 invited presentations
12:50-15:00	*lunch break*
15:00-17:00	6 invited presentations
17:00-17:20	*coffee break*
17:20-19:00	5 invited presentations
19:00-20:30	*break*
20:30-22:00	*dinner*

Tuesday, 12 June 2001
2 sessions dedicated to Prof. A. Acrivos

09:00-10:40	5 invited presentations
10:40-11:00	*coffee break*
11:00-12:00	plenary presentation by Prof. A. Acrivos
12:00-14:00	*lunch break*
14:00-15:30	6 presentations
15:30-16:00	*coffee break*
16:00-17:15	5 presentations
17:15-17:45	*coffee break*
17:45-19:00	5 presentations
19:00-20:30	*break*
20:30-22:00	*dinner*

Wednesday, 13 June 2001

08:00-14:00	*Trip to Olympia and lunch*
14:00-15:00	*Return from Olympia*
15:00-17:00	*break*
17:00-18:30	6 presentations
18:30-19:00	*coffee break*
19:00-20:30	6 presentations
20:30-21:00	*break*
21:00-22:30	*conference dinner*

Thursday, 14 June 2001

08:30-10:15	7 presentations
10:15-10:45	*coffee break*
10:45-12:15	6 presentations
12:30-14:00	*lunch break*

14:00-15:00	4 presentations
15:00-15:30	*coffee break*
15:30-17:00	6 presentations
17:00-17:15	*closing remarks*

Total:

25 invited presentations by people affiliated with Prof. A. Acrivos (20 minutes each one)
Plenary presentation by Prof. A. Acrivos (1 hour)
51 oral presentations (15 minutes each one)
13 Posters

Monday, 11 June 2001

08:30 Registration

09:00 Welcome Remarks

Morning session I: Dedicated to Prof. A. Acrivos, “Suspensions and particulates”

09:30 **J.D. Goddard**
Material instability and stress localization

09:50 **D. Barthès-Biesel**, A. Diaz
Capsule motion in flow: role of membrane rheology

10:10 T. Loimer, **A. Nir**, R. Semiat
Shear-induced corrugation of free interfaces in concentrated suspensions

10:30 Leonard F. Pease III, **W.B. Russel**
Linear stability analysis of thin leaky dielectric films subjected to electric fields

10:50 **R.H. Davis**, Y. Wu, A.Z. Zinchenko
Dynamic simulations of emulsion rheology

11:10 coffee break

Morning session II: Dedicated to Prof. A. Acrivos, “Suspensions and particulates”

11:30 **J.F. Brady**, I. Carpen
Second normal stress jump instability in non-Newtonian fluids

11:50 **F.A. Gadala-Maria**
Shear-induced anisotropy in suspensions of spheres: causes and consequences

12:10 **W.L. Olbricht**, B.W. Roberts
Flow of dilute suspensions in capillary networks

12:30 **N.J. Wagner**
Mechanism of reversible shear thickening in colloidal dispersions

12:50 end

Afternoon session I: Dedicated to Prof. A. Acrivos, “Polymer dynamics”

15:00 **L. Gary Leal**, G. Sgalari, J.J. Feng
Computational studies of the dynamics of liquid crystalline polymer in shear flows

15:20 G. Ianniruberto, **G. Marrucci**

A simple constitutive equation for entangled polymers incorporating CCR and chain stretching

15:40 **G.G. Fuller**
Rheology in two dimensions

16:00 **L.A. Archer**
Friction and dynamics of entangled polymer liquids

16:20 **J. P. Oberhauser,** L.Gary Leal
Rheo-optical experiments and modeling of entangled polymer solutions: Steady and transient flows

16:40 **C.J.S. Petrie**
Pure shear or planar extension, which name is misleading?

17:00 coffee break

Afternoon session II: Dedicated to Prof. A. Acrivos, "Newtonian fluid mechanics"

17:20 K. Sarkar, **W.R. Schowalter**
Behavior of a free jet formed from an emulsion of two Newtonian fluids

17:40 **R. Mauri**
Two-dimensional model of phase segregation in liquid binary mixtures with an initial concentration gradient

18:00 **G.S. Triantafyllou**, L. Shen, D.K.P. Yue
Mixing of a passive scalar near a free surface

18:20 **N.A. Pelekasis**, D.N. Smyrnaios, J.A. Tsamopoulos
Stratified boundary layer flow of a gas stream and a liquid
film past solid surfaces

18:40 **S. Kim**
Fluid Mechanics and Rheology Research Opportunities in Pharmaceutical R&D Technologies

19:00 end

Tuesday, June 12 2001

Morning Session I: Dedicated to Prof. A. Acrivos, “Non-Newtonian fluid mechanics”

09:00 **J.R.A. Pearson**
Models for flow of non-Newtonian fluids through porous media

09:20 **R.I. Tanner**
A suspension model for polymer solidification rheology

09:40 S. Nigen, **K. Walters**
Viscoelastic contraction flows: Comparison of axisymmetric and planar configurations

10:00 **J-M. Piau**
Viscoplastic Boundary Layers

10:20 B.T. Liu, S. J. Muller, **M.M. Denn**
Convergence of a regularization method for flow of a Bingham material past a sphere

10:40 coffee break

Morning Session II

11:00 **A. Acrivos**
Particle migration and segregation in suspension flows undergoing shear

12:00 end

Afternoon Session I: Polymer rheology

14:00 M.E. Mackay, M. Jeong, R. Vestberg, C.J. Hawker
Rheology of dendrimers and their hybrid copolymers with linear polymers

14:15 A. Véron, A.F. Martins
Combining NMR and classical rheometry to evaluate the viscoelastic properties of main-chain nematic LC polymers

14:30 L. Braun-Shmueli, O. Netanel, O. Regev, M. Gottlieb
Microemulsions of ABA amphiphilic block copolymers and surfactants

14:45 A. Romoscanu, M.B. Sayir, K. Häusler, I. Roberts
High frequency dynamical viscometry on confined emulsions

15:00 C. Tsitsilianis
Telechelic polyelectrolytes: New developments in the rheology of aqueous formulations

15:15 A. Zupančič, U. Florjančič, M. Žumer

Viscoelasticity and network structure of water-based polysaccharide systems

15:30 coffee break

16:00 A.D. Gotsis
Elongational rheology of branched polypropylene

16:15 D. Vlassopoulos, T. Pakula
Relaxational mechanisms in hyperstar melts

16:30 C. Toprakcioglu, D. Anastassopoulos, A. Vradis, A. Papayianopoulos, S. Baker, A. Menelle
Polymer brushes under strong shear flow in a good solvent

16:45 S. H. Anastasiadis, H. Retsos
Block copolymers as emulsifiers in homopolymer blends: effects of additive MW, architecture, and composition

17:00 E. Kontou, G. Spathis
Theoretical and experimental investigation of non-linear viscoelastic and viscoplastic response of amorphous polymers

17:15 coffee break

Afternoon Session II: Drops and particulates

17:45 M. Carin, C. Postel, M. Rachik, D.Barthès-Biesel
Determination of the rheological properties of microcapsules

18:00 W. Lin, A. Kaiser, A.L. Graham, M.S. Ingber
The influence of walls on particle migration in suspensions

18:15 P. Vlahovska, J. Blawzdziewicz, M. Loewenberg
Dynamics of deformable surfactant-covered drops

18:30 P. Perona, S. Sordo
Effects of turbulent motion on breakdown processes of natural fibers

18:45 A.G. Papathanasiou, A.G. Boudouvis
Three-lobed shape formation of captive ferrofluid drops

19:00 end

Wednesday, June 13 2001

Morning Session: Visit to Olympia

08:00 Visit to Olympia Archeological site and lunch

15:00 Return from Olympia

Afternoon Session I: Suspensions and colloids

17:00 D. De Kee, L. Zhu, K. Papadopoulos
Static yield stress measurements of suspensions

17:15 R.R. Huilgol
Variational inequalities in viscoplastic fluids – Theory & applications

17:30 B. Abu-Jdayil, P.O. Brunn
The behavior of electrorheological fluids in torsional flow

17:45 T. Aubry, F. Bossard, M. Moan
Influence of macromolecular associations on the dilute properties of a clay suspension

18:00 E. Stiakakis, D. Vlassopoulos, G. Fytas, A. Rissanou, I.A. Bitsanis
Gelation phenomena in soft colloidal spheres

18:15 T. Lyashenko, V. Voznesensky, Y. Ivanov
Modeling the influence of mix proportions on correlation between destruction pace and thixotropy of suspensions

18:30 coffee break

19:00 P.K. Rozakeas, R.J. Snow
Electrokinetically enhanced flow of coal-water suspensions in pipes

19:15 T.B. Goudoulas, E.G. Kastrinakis, S.G. Nychas
Rheology of dense lignite-water suspensions; preshearing and transition stresses

19:30 L. Mondy, R. Rao, R. Lagasse, M. Hopkins, S. Altobelli, M. Ingber, A. Mammoli, D. Fang
Modeling shear induced particle migration

19:45 K. Sadeghy, S. Salimi, M. Khairandish
The effects of pressure and temperature on the wall slip phenomenon of drilling muds

Afternoon Session II: Bio-rheology

20:00 C. G. Provatidis
Two-dimensional FEM creep analysis of orthodontic tooth movement

20:15 M. Barracó-Serra
Viscometrical behavior of systems with dermathologic and cosmetic applications

20:30 end

Thursday, June 14 2001

Morning Session I: Computational rheology

08:30 C. M. Chiujdea
Nonlinear dynamics of dilute polymer solutions

08:45 K. Atalik, R. Keunings
A temporal nonlinear stability analysis of viscoelastic channel flows

09:00 G. Georgiou, P. Lemenn, A. Alexandrou
Numerical simulations of generalized Newtonian flows involving two free surfaces

09:15 M.V. Apostolakis, V.G. Mavrantzas, A.N. Beris
Stress-induced migration effects on the Taylor-Couette flow of a dilute polymer solution

09:30 L. Saudi, N. Zeraibi
Numerical simulation of the planar contraction flow of the Oldroyd-B fluid

Morning Session II: Polymer processing

09:45 E. Mitsoulis, M. Beaulne, D. Kammer, A. Zissis
Modeling of viscoplastic lid-driven cavity flow using finite element simulations

10.00 J. Vlachopoulos, C. Bellehumeur, M. Kontopoulou
Particle sintering and melt densification in rotational molding

10:15 coffee break

10:45 C. Jeggy, F. Dupret
Viscoelastic modeling of micro-injection moulding

11:00 A.B. Ariawan, S.G. Hatzikiriakos
Rheology of polytetrafluoroethylene in paste extrusion

11:15 L. Slemenik, A. Zupančič, M. Žumer
The influence of complex rheological properties on mixing

11:30 E.C. Achilleos, K.N. Christodoulou, I.G. Kevrekidis
Dynamical process of polyelectrolyte gel swelling - Swelling controlled solute release

11:45 J. den Doelder
Multi-scale thermoplastic foam rheology modeling

12:00 D. Giannakidis
MORNOS: A leading Greek plastics packaging company

12:15 end

Afternoon Session I: Complex Newtonian fluid flow

14:00 M. Vlachogiannis, N. Malamataris, V. Bontozoglou
Solitary wave dynamics of Newtonian film flows: Experiment and simulation

14:15 Ch. Kouris, J.A. Tsamopoulos
Two-phase flow in an undulating tube: Transitions from stratified to discontinuous flow of one of the fluids

14:30 D.P. Pazis, N.A. Malamataris
Analyzing Acrivos' experiments with finite elements

14:45 D. Jankovic, A.N. Beris, R. Keunings, G.S. Winckelmans
Low Reynolds number turbulent channel flow

15:00 coffee break

Afternoon Session II: Theory and modeling

15:30 J.A. Pathak, R. Kant, S.K. Kumar, R.H. Colby
Double reptation predictions of the linear viscoelasticity of melt miscible polymer blends

15:45 A.E. Likhtman, T.C.B. McLeish
Quantitative theory for linear rheology of linear entangled polymers

16:00 M. Hütter, H.C. Öttinger
A GENERIC formulation of two-phase flow

16:15 C. Tsenoglou
Non-Newtonian rheology of entangled polymer solutions and melts

16:30 J. de Joannis, J. Jimenez, R. Rajagopalan, J. Thomatos, I.A. Bitsanis
Chain conformations and forces in physisorbed layers of homopolymer colloid stabilizers: Comparison between Monte Carlo and mean field predictions

16:45 V.A. Harmandaris, V.G. Mavrantzas, D.N. Theodorou
Prediction of the rheological properties of long polyethylene melts via atomistic molecular dynamics simulations

17:00 closing remarks

17:15 end

Poster Session

1. E. Lac, N.A. Pelekasis, J.A. Tsamopoulos, D. Barthès-Biesel
   Mechanical properties and behavior of capsules in 3d flows

2. E. Mitsoulis, G. Athanasopoulos
   Modeling of viscous effects in blade coating flows

3. A. Harkati, M. Drir, D. Ouadjaout, R. Younsi
   Fluid flow and heat transfer during liquid encapsulated Czochralski crystal growth of III-V compound semiconductors

4. R. Younsi, A. Harkati, D. Kalache
   Numerical simulation of heat and mass transfer in trapezoidal porous cavity

5. L. Achab, S. Benhadid
   Numerical simulation of blood flow through stenotic artery

6. F. Iachachene, S. Benhadid
   Analytic solution for the analysis of flow in an elastic artery

7. I. Katsambas, C. Tsitsilianis
   Rheological properties of heterotelechelic polyelectrolytes in aqueous media

8. G. Bokias, Y. Mylonas, G. Staikos, D. Hourdet, I. Iliopoulos, G.G. Bumbu, C. Vasile
   Temperature and shear induced thickening properties of aqueous solutions of n-isopropylacrylamide-based polymers

9. M. S. Valavanides, A.C. Payatakes
   Steady-state fully-developed two-phase flow in porous media: Mechanistic model and a conjecture concerning the underline principle

10. L. Achab, S. Benhadid
    Non-Newtonian behavior flow through arterial stenosis

11. L. Hilliou, A.G. Feio, A.F. Martins, D. Collin, P. Martinoty
    Viscoelastic flow behavior of a side-chain nematic LC polyacrylate

12. N. Kherfellah, K. Bekkour, S. Hamza, M. Khodja, S. Benhadid
    Static and dynamic filtration properties of polymers in water-based drilling muds

13. F. Greco
    Slow flows of a non-Newtonian drop in a non-Newtonian fluid

INVITED LECTURES

MATERIAL INSTABILITY AND STRESS LOCALIZATION

J. D. GODDARD

Department of Mechanical and Aerospace Engineering
University of California, San Diego
9500 Gilman Drive
La Jolla, CA 92093-0411 USA

Material or constitutive instability pertains to the instability of spatially homogeneous states. As pointed out in a recent comprehensive review [1], the phenomenon is embodied in a number of constitutive models, which appear to account for the appearance of various patterned states involving "strain localization", e.g. shear banding and necking, in diverse materials. The prototypical instability can often be traced to non-monotone stress-deformation behavior, such as "shear thinning" or "strain softening", or to a more general "loss of static ellipticity", resulting in ill-posedness and Hadamard instability in the field equations [1].

One can envisage the possibility of another type of instability or "blowup" in the field equations associated with extreme "strain hardening" and multiplicity of stress states, which also might lead to patterned states, but now involving "stress localization". Some possible examples, with early references, are:

1."coil-stretch" transitions in polymer fluids [2],
2. stress multiplicity ("ignition-extinction") in gas-solid dispersions at high Stokes number [3],
3."micro-arching", force chains and (mathematical) "hot spots" in granular media [4], [5], and
4."discontinuous-dilatant" behavior and force-percolation clusters in sheared suspensions [6], [7].

The present article provides a comprehensive review and synthesis of these and more recent works, together with a tentative and qualitative mathematical framework for describing the associated instability.

REFERENCES:

1. Goddard, J.D. & Alam, M. 1999 "Shear-Flow and Material Instabilities in Particulate Suspensions and Granular Media", *Particulate Sci. Tech.,* **17**, 69.
2. de Gennes, P. -G. 1974 "Coil-stretch transition of dilute flexible polymers under ultrahigh velocity gradients, *J. Chem.Phys.*, **60**, 5030.
3. Sangani, A.S. et al. 1996 "Simple shear flows of dense gas-solid suspensions at finite stokes number", *J. Fluid Mech.*, **313,** 309**.**
4. Drescher, A. 1972 "Photoelastic Verification of a Mechanical Model for the Flow of a Granular Medium", *J. Mech.Phys Solids,* **20**, 337.
5. Hill, J.M. 2000, "Similarity 'hot-spot' solutions for a hypoplastic granular medium", *Proc. Roy. Soc. Lond.* A, **456**, 2653.
6. Hoffman. R.L., 1972 "Discontinuous and dilatant viscosity behavior in concentrated suspensions.I. Observation of a flow instability.", *Trans. Soc. Rheology*, **16**, 155.
7. Brady, J.F. & Bossis, G. 1985, "The rheology of concentrated suspensions of spheres in simple shear flow by numerical simulation", *J. Fluid Mech.,* **155, *105***

CAPSULE MOTION IN FLOW: ROLE OF MEMBRANE RHEOLOGY

D. BARTHÈS-BIESEL, A. DIAZ

UMR CNRS 6600, UTC, BP 20529, 60205 Compiegne, France

A capsule consists of an internal medium (pure or complex liquid), enclosed by a deformable membrane that is usually semi-permeable. Capsules are frequently met in nature (cells, eggs) or in industrial processes (biomedical, pharmaceutical, cosmetic or food industry). The membrane is usually so thin that it is approximated by an elastic or viscoelastic 2D surface isotropic in its plane. If only small deformations are involved, a linear 2D Hooke law is appropriate. In the domain of large deformations, more complex membrane constitutive law must be considered. For example, a biocompatible gelatine membrane may be treated as a thin sheet of a volume incompressible material. This leads to a Mooney-Rivlin law. Polymerised interfaces and bilayers are well described by a law, introduced by Skalak, that accounts separately for the shear deformation and for the area dilatation of the material. Obviously the membrane rheology will determine the capsule behaviour.

Correspondingly, we study the motion and deformation of capsules with different types of membrane, when they are freely suspended in a shear flow. Two free surface flow problems (motion of the internal liquid and of the suspending fluid) and a solid mechanics problem (deformations of the membrane) must be solved simultaneously. An efficient method consists in recasting the Stokes equations in integral form and in using the boundary integral technique. Results will be presented for different flow configurations, such as an axisymmetric pure straining flow and the flow of a capsule through a small pore.

SHEAR-INDUCED CORRUGATION OF FREE INTERFACES IN CONCENTRATED SUSPENSIONS

T. LOIMER, A. NIR, R. SEMIAT

Department of Chemical Engineering, Technion
Haifa 32000, Israel

When a concentrated suspension of small inertia-less particles in a viscous fluid is sheared between two parallel belts a free surface exists with a direction orthogonal to the plane of the simple shear flow. We observed a development of corrugation on this surface. The corrugation appears as an ensemble of disturbances driven by shear-induced diffusion and restrained by surface forces. The roughness of the surface disturbances depends on the particle size, on particle concentration and on the fluid surface tension. The corrugation has many frequencies with scales ranging from particle size to an order of magnitude larger. The latter appear in the form of waves traveling with the local surface fluid speed.

In this communication we present a report on the phenomenon and its dependence on the physical parameters. A qualitative description is presented and the dimensionless groups governing the extent of the shear-induced corrugation are defined. We introduce the notion of a macroscopic effective surface tension, which depends on the surface particle concentration. The influence on the stability of the surface is examined and discussed.

LINEAR STABILITY ANALYSIS OF THIN LEAKY DIELECTRIC FILMS SUBJECTED TO ELECTRIC FIELDS

LEONARD F. PEASE III, WILLIAM B. RUSSEL

Department of Chemical Engineering
Princeton University
Princeton NJ 08544-5263
USA

An intriguing process, known as lithographically induced self assembly (LISA)[1,2], is initiated by positioning a planar or patterned template parallel to and within 100 nm or less of a flat silicon wafer coated with a thin film of poly(methyl methacrylate), for example, and then raising the temperature above the glass transition/melting temperature of the film. Electric fields that arise naturally from the contact potentials of the various interfaces[3] or are imposed externally[4] exert a force on charges induced at the polymer-air interface, thereby reducing the pressure in the film below atmospheric. If all surfaces are flat and parallel, the static equilibrium that results is unstable to disturbances with wavelengths for which the electrostatic force overcomes the capillary pressure generated by curvature. If the upper surface is patterned discontinuously, the film is unconditionally unstable at edges and corners of the template. In either case, flow ensues, generating a pattern in the film with form and periodicity reflecting both the geometry of the template and the characteristic length of the instabilityThough the initiation of the process as outlined above is clear qualitatively, the forces guiding the evolution of the film into the remarkably periodic microstructures observed are not. Our goal here is to create a sound understanding of the mechanism through quantitative modeling to facilitate the conversion of these microstructures into nanostructures. Given the apparent importance of conductivity in the film we adopt the "leaky dielectric model",[5,6] which also allows for redistribution of charges on the interfaces, and undertake a linear stability analysis to explore the complex dependence of the phenomena on the various process parameters with particular attention to the conductivity and the film thickness.

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DYNAMIC SIMULATIONS OF EMULSION RHEOLOGY

ROBERT H. DAVIS, YINGYUAN WU, ALEXANDER Z. ZINCHENKO

Department of Chemical Engineering
University of Colorado
Boulder, CO 80309-0424

Several numerical simulations of the rheology of an emulsion of drops of one fluid immersed in a second, immiscible fluid are described for viscous fluids at low Reynolds number. The first approach considers concentrated emulsions of deformable drops undergoing either sedimentation or simple shear flow. A hybrid of economical multipole [1] and boundary-integral [2] techniques is applied to $N = 0(100)$ deformable drops in a triply periodic box. For sedimentation, the average drop velocity increases with time due to deformation-induced clustering, if the drop volume fraction is not too high [3]. For shear flow, significant shear thinning is observed due to deformations, and the second normal stress difference is negative while the first normal stress difference changes from negative to positive with increasing capillary number [4]. At very small capillary numbers, the drops are nearly spherical and the hybrid algorithm, even with two-orders of magnitude gain over full boundary-integral simulations, is too difficult at large volume fractions, due to prohibitively small time steps and insufficient resolution in the small gap regions. Thus, a new algorithm was developed for simulations of spherical drops, following earlier work on effective conductivity using economical multipole techniques, matched asymptotic expansions and Wigner functions [5]. Finally, an approximate simulation method, capable of describing complex flows of dilute emulsions of deformable drops, is described by approximating the drop shapes as ellipsoids.

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SECOND NORMAL STRESS JUMP INSTABILITY IN NON-NEWTONIAN FLUIDS

J. F. BRADY, I. CARPEN

Division of Chemistry and Chemical Engineering
California Institute of Technology
Pasadena, CA 91125

An instability mechanism is shown to operate in complex, non-Newtonian fluids in which a jump in normal stresses occurs between two fluids. Fluids with a negative second normal stress difference can be unstable with respect to transverse or spanwise perturbations. The mechanism appears to be generic, although the details will depend on the specific flow and the nature of the complex fluid. The instability mechanism is illustrated for falling film flow and two-layer Couette flow of viscous suspensions.

SHEAR-INDUCED ANISOTROPY IN SUSPENSIONS OF SPHERES: CAUSES AND CONSEQUENCES

FRANCIS A. GADALA-MARIA

Department of Chemical Engineering, University of South Carolina, Columbia, SC 29208

This paper reviews the progress in understanding the shear-induced anisotropy in concentrated suspensions of spheres from the time of the publication of the paper by Gadala-Maria and Acrivos (*J. Rheol. 24*, 799-814, 1980) to the present. In particular, work at the University of South Carolina, including the recent evidence of a transition in the normal forces in the suspension upon a reversal of the direction of shear will be presented.

Based on shear stress measurements, Gadala-Maria and Acrivos concluded that non-colloidal particles suspended in a Newtonian fluid acquire an anisotropic structure when subjected to steady shear. They found that the shear stress in a concentrated suspension behaved differently depending on the direction of previous shear. It attained its steady state value nearly instantaneously when, after a period of rest, shear was restarted in the same direction but underwent a characteristic strain-dependent transition when shear was restarted in the opposite direction.

Later, visual observations by Parsi quantified these anisotropic structures and showed that, as expected, the structures resulting from shear in one direction were mirror images of those resulting from shear in the opposite direction. Kim manufactured anisotropic composites by curing sheared suspensions of glass beads in solutions of unsaturated polyester and styrene and characterized their structure. Under steady shear, the anisotropic structures that developed were fairly independent of the type of particle used and of the rheology of the suspending fluid. Under oscillatory shear, however, the anisotropic structures depended strongly on the rheology of the suspending fluid and on the amplitude, frequency, and duration of the oscillatory shear.

Recently, Kolli was able to measure transitions in the normal force from a concentrated suspension of spheres sheared between parallel rings. The normal force grew quickly from zero to its steady state value when the suspension was sheared in the same direction as that of previous shear. However, when shear was restarted in the opposite direction the normal force started at a negative value and gradually grew to its steady state positive value. The possible causes of the observed anisotropy and the information that may be gleaned from the transitions in both the shear stress and the normal stresses will be discussed.

FLOW OF DILUTE SUSPENSIONS IN CAPILLARY NETWORKS

W.L. OLBRICHT, B.W. ROBERTS

School of Chemical Engineering
Cornell University
Ithaca, NY 14853 USA

Experimental results are presented for the low Reynolds number flow of a dilute suspension of neutrally buoyant rigid spheres in capillary networks. The motion of suspensions in capillary networks is relevant to such problems as microcirculatory blood flow, multiphase flow in porous media, and flow in multiphase microfluidic systems. One of the important features of these examples is the way in which the flow affects the distribution of the particles among the branches of a capillary network. Experimental observations have shown that the distribution of particles among the branches of a capillary network often is highly inhomogeneous in these situations. Furthermore, the particle distribution fluctuates in time throughout the network and along the length of an individual capillary segment.

The way particles distribute throughout a capillary network is influenced not only by the motion of particles within individual branches, but also by the partitioning of particles at divergent bifurcations. A divergent bifurcation is a junction where a capillary splits to form two capillaries. It is well known that the partitioning of particles between the downstream branches of a bifurcation can differ from the partitioning of total volume (particles + suspending fluid) between the branches. The difference between the fraction of particles entering a given downstream branch and the fraction of total volume entering the same branch can be substantial, especially when the diameter of the particles is comparable to the diameter of the branch tubes.

We have measured experimentally the partitioning of particles at divergent bifurcations for a wide range of conditions. The parameters that we have varied include the size of the particles relative to the capillary diameter, the angles between the downstream branches of the bifurcation, and the relative diameters of the bifurcation branches. We have also varied the volume fraction of particles. Results show that partitioning of particles at bifurcations in some circumstances is strongly affected by the detailed shape of the bifurcation. Furthermore, partitioning of particles is influenced by interactions among the particles for surprisingly small values of the particle volume fraction. Indeed, the flux of particles at a bifurcation is affected by two-particle interactions for volume fractions as low as 0.02.

The experimental data are used in macroscopic momentum balances to predict the motion and distribution of particles in relatively simple capillary networks. The momentum balances combine estimates from various sources in the literature for the hydraulic resistance caused by the presence of the particles with the present results for particle partitioning at bifurcations. Even in relatively simple capillary networks, the models reproduce, at least qualitatively, mechanisms that lead to inhomogeneous particle distributions. The results suggest ways to use flow at bifurcations to control the motion of particles in multiphase microfluidic systems, and, if desired, to separate particles from the fluid in which they are immersed.

MECHANISM OF REVERSIBLE SHEAR THICKENING IN COLLOIDAL DISPERSIONS

NORMAN J. WAGNER

Center for Molecular and Engineering Thermodynamics, Dept. of Chemical Engineering,
University of Delaware, Newark, DE 19716 USA

The particle size dependence of the reversible shear thickening transition in dense colloidal suspensions is explored. Five suspensions of monodisperse silica are synthesized via the Stöber synthesis. The physicochemical properties of the dispersions are quantified using TEM, DLS, SANS, electrophoresis, and several viscometry techniques. Rheology measurements indicate a critical stress marking the onset of reversible shear thickening that depends on the dispersion's particle size, concentration, polydispersity, and interparticle interactions. A simplified two-particle force balance between the interparticle repulsive forces and the hydrodynamic compressive forces is used to derive a scaling relationship between this critical shear stress and the suspension properties. The scaling is tested against the fully characterized silica dispersions, which span over a decade in particle size. Furthermore, bimodal mixtures of the dispersions are employed to evaluate the accuracy of the scaling to predict the critical shear stress for dispersions with varying degrees of polydispersity. The success of the scaling supports the hydrocluster mechanism for shear thickening and suggests methods for controlling shear thickening by tailoring particle properties.

COMPUTATIONAL STUDIES OF THE DYNAMICS OF LIQUID CRYSTALLINE POLYMER IN SHEAR FLOWS

L. GARY LEAL[1], GIORGIA SGALARI[1], JIMMY J. FENG[2]

[1]Dept. of Chemical Engineering, Univ. Of California at Santa Barbara
[2]Levich Institute, City College of CUNY, New York, New York 10031

We address the problem of structure formation in the flow of liquid crystalline polymers by means of numerical solutions based on theoretical models of the LCP. The work primarily utilizes the molecular model theory of Doi, both in its original monodomain form, and also via a generalization that incorporates distortional elasticity by means of a non-local nematic potential proposed recently by Marrucci and Greco. The computations also use a corresponding expression for the bulk stress that was derived in a recent paper from our group (Feng et al J. Rheol. **44,** 1085(2000)).

The goal of our simulations is to explore the evolution of the LCP structure and flow, as predicted by this theory, including the possibility of in-plane tumbling instabilities, out of plane tipping of the director and the formation of disclinations leading to a final polydomain structure. However, the calculations to date are mainly limited to planar flows.

We also present recent calculations using the well-known Leslie-Erickson approximation of the full Doi/Marrucci-Greco model to address fully three-dimensional flow structures that occur in a "simple shear" device due to the onset of instabilities leading to the formation of roll cells aligned in the primary flow direction, and to further explore the mechanism for onset of disclinations in this case.

A SIMPLE CONSTITUTIVE EQUATION FOR ENTANGLED POLYMERS INCORPORATING CCR AND CHAIN STRETCHING

G. IANNIRUBERTO, G. MARRUCCI

University Federico II, Piazzale Tecchio, Napoli, Italy

In recent times the well known Doi-Edwards theory for entangled polymers has been augmented by including the mechanism of convective constraint release (CCR) [1, 2], which improves on the problem of excessive shear thinning at moderate to high shear rates predicted by the classical theory. Mead et al.[3] have proposed a model that also accounts for chain stretching, which takes place at even higher shear rates, i.e., in flows faster than the reciprocal Rouse time. Here we present a different way of accounting for chain stretching, based on considerations previously developed for a simple dumbbell model [4]. Without adding further parameters to the basic CCR model [2], the constitutive equation proposed here seems to predict correctly the nonlinear rheological response in a variety of situations, ranging from step strains to transient and steady shear and elongational flows.

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RHEOLOGY IN TWO DIMENSIONS

GERALD G. FULLER

Department of Chemical Engineering
Stanford University
Stanford, CA 94305-5025

The dynamics of fluid/fluid interfaces control a wide range of phenomena of technological and biological interest. These include flow-induced deformation of blends, emulsions and foams, and cell division in biology. In many applications, amphiphiles can collect at these interfaces and strongly and render the interfacial rheology non-Newtonian. As a result, the fluid mechanical response of films as thin as a monolayer can be highly nonlinear. This paper presents experimental results combining mechanical and optical measurements to reveal the microstructural origins of a variety of phenomena.

Several examples are presented in this paper: the problem of order-disorder in a two-dimensional liquid crystal, the non-Newtonian fluid mechanics of a high molecular weight, flexible polymer chain laying flat on an interface, and the dynamics of two-dimensional suspensions. In the first example, it is demonstrated that many monolayer systems spontaneously order into liquid crystalline domains due to the extra constraints that pin molecules to the interface. It is demonstrated that both thermotropic and lyotropic order-disorder transitions can occur. This is accomplished using a combination of mechanical and optical measurements of orientation. The experiments involving a flexible polymer amphiphile involve surface flows through contractions and demonstrate that these monolayer systems undergo highly nonlinear flow phenomena that are reminiscent of their 3D counterparts. Finally, the dynamics of two-dimensional suspensions are examined. These systems are formed from monolayers of monosized latex spheres pinned at either the air/water or oil/water interfaces. Under appropriate conditions highly organized, two-dimensional crystals are formed that are subjected to both shear and extensional flows. These are examined using flow-microscopy methods as well as interfacial stress rheometry.

FRICTION AND DYNAMICS OF ENTANGLED POLYMER LIQUIDS

LYNDEN A. ARCHER

Cornell University, School of Chemical Engineering, Ithaca NY 14853

The equilibrium structure and relaxation dynamics of uncharged, flexible macromolecules near solid substrates are widely believed to be different from those in bulk polymer liquids. Substrates are for instance credited with reducing configurational freedom, inducing density fluctuations, and altering molecular relaxation dynamics of polymer chains located within a few molecular diameters of the polymer/substrate interface. While the practical importance of such surface effects are easily appreciated, fundamental consequences for polymer processing and rheometry are not. In this presentation various aspects of polymer dynamics near surfaces will be discussed. I will focus in particular on the effect of a tightly bound surface layer on dynamic friction between surface and bulk polymer chains. I will show how theories of molecular friction near interfaces can be generalized to describe entanglement friction in bulk polymer liquids. Applications to rheology of linear polymer liquids under fast flow conditions, viscoelasticity of bidisperse linear homopolymer and star/linear blends, and relaxation dynamics of multiarm pom-pom polymers will be discussed.

RHEO-OPTICAL EXPERIMENTS AND MODELING OF ENTANGLED POLYMER SOLUTIONS: STEADY AND TRANSIENT FLOWS

JAMES P. OBERHAUSER[1], L. GARY LEAL[2]

[1]Department of Chemical Engineering, University of Virginia, Charlottesville, VA 22904
[2]Department of Chemical Engineering, University of California, Santa Barbara, Santa Barbara, CA 93106

Understanding the physics of entangled polymer solutions and melts under flow is critical to a variety of processing applications. Despite a tremendous research effort on these materials, no models are successful in predicting optical and mechanical properties under all flow conditions. The Doi-Edwards reptation model, being of molecular rather than constitutive origin, has the broadest appeal; however, even it suffers from flaws such as excessive shear thinning, which leads to a shear stress maximum as the strain rate increases. Furthermore, the nonlinear viscoelastic regime, which is most relevant to industrial applications, is poorly represented by most models.

We will present experimental flow birefringence data for entangled polystyrene solutions in both shear and more extensional-type flows along with comparisons with versions of the reptation model with non-linear chain stretching (known as the DEMG model). The steady state results for the average orientation angle suggest that the DEMG model generates more orientation with the flow direction than experiments seem to indicate, which is consistent with the excessive shear thinning observed. Other researchers have proposed mechanisms (convective constraint release, chain length fluctuations, etc.) by which the microstructure may be affected by flow in such a way as to reduce the effective reptation time, leading to less orientation and better quantitative predictions.

The effect of these enhanced relaxation mechanisms on steady and transient shear flows (including startup from rest, step shear, and reversing shear) will be discussed. Comparisons with experimental data show that these mechanisms improve predictions for the orientation angle but still fall short in some circumstances.

PURE SHEAR OR PLANAR EXTENSION, WHICH NAME IS MISLEADING?

CHRISTOPHER J S PETRIE

Department of Engineering Mathematics,
University of Newcastle upon Tyne, UK.

The two-dimensional flow in which a fluid is sheared equally in two perpendicular directions is described as "pure shear" (i.e. shear without vorticity) or as "planar extension" (with equal and opposite strain rates in two perpendicular directions). For a Newtonian liquid the terminology does not hold any great significance, but for polymeric liquids (or any other liquids) whose behaviour in shear is radically different from behaviour in extension, the question does arise as to whether the flow is best described as a shearing flow or an extensional flow. A new perspective on this problem is given by the consideration of so-called exponential shear (strain rate increasing with time) and also of extensional flow with a strain rate reducing with time (constant velocity extension).

This note sets out to clarify the issues in the light of some recent work (Kwan, Woo and Shaqfeh, 2001). There are two classic sets of experiments which address the question (Zülle, Linster, Meissner and Hürlimann, 1987; Samurkas, Larson and Dealy, 1989) and more recently Venerus (2000) has published experimental results and a discussion of the problem. Among the key issues are the significance of vorticity, what we mean by "steady flow", whether a flow like exponential shear should be regarded as "weak" or "strong" and what sort of constitutive equation is going to be needed to describe the observed behaviour (or that predicted by simulation using a molecular or microstructural model). Indeed, this last remark raises the question of how much we can say independently of an assumed constitutive model (or at least a constitutive presupposition).

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BEHAVIOR OF A FREE JET FORMED FROM AN EMULSION OF TWO NEWTONIAN FLUIDS

KAUSIK SARKAR, W. R. SCHOWALTER

Department of Chemical Engineering, University of Illinois at Urbana-Champaign
Urbana, IL 61801, USA

It is known from experiments published more than ten years ago that an emulsified liquid undergoes a large expansion when exiting from a conduit into a third liquid immiscible with the components of the emulsion. The physics governing this phenomenon have not been resolved. In the present work we consider the role played by relaxation of the emulsified droplets as they exit a conduit and form a free jet. The role of interfacial tension during this process imposes a characteristic relaxation time, thus drawing a parallel to behavior of viscoelastic jets. Through computational modeling one is able to determine the importance of interfacial tension on the experiments cited above. A boundary element method has been employed. This requires special features to deal with microscopic and macroscopic aspects of free boundaries.

TWO-DIMENSIONAL MODEL OF PHASE SEGREGATION IN LIQUID BINARY MIXTURES WITH AN INITIAL CONCENTRATION GRADIENT

ROBERTO MAURI

Department of Chemical Engineering, DICCISM, University of Pisa, 56126 Pisa, Italy

We simulate the phase segregation of a deeply quenched binary mixture with an initial concentration gradient. Our theoretical model follows the standard model *H*, where convection and diffusion are coupled via a body force, expressing the tendency of the demixing system to minimize its free energy. This driving force induces a material flux much larger than that due to pure molecular diffusion, as in a typical case the Peclet number, expressing here the ratio of thermal to viscous forces, is of order 10,000. Integrating the equations of motion in 2D, we show that the behavior of the system depends on the values of the Peclet number and the non-dimensional initial concentration gradient. In particular, the morphology of the system during the separation process reflects the competition between the capillarity-induced drop migration along the concentration gradient and the random fluctuations generated by the interactions of the drops with the local environment. For large values of the Peclet number, the nucleating drops grow with time, until they reach a maximum size, whose value decreases as the Peclet number and the initial concentration gradient increase. This behavior is due to the fact that the nucleating drops do not have the chance to grow further, as they tend to move towards the homogeneous regions where they are assimilated.

MIXING OF A PASSIVE SCALAR NEAR A FREE SURFACE

G. S. TRIANTAFYLLOU[1], L. SHEN[2], D. K. P. YUE[2]

[1]Department of Naval Architecture and Marine Engineering,
National Technical University of Athens, Zografou Campus, 15773, Athens, Greece
Department of Ocean Engineering, Massachusetts Institute of Technology,
Cambridge, Massachusetts 02139

The mixing of a passive scalar in shear flow with a free surface is a problem that one encounters in many applications. Examples include the spreading of pollution and heat near a free surface. The free surface influences the turbulent mixing with two different mechanisms: (i) Through the reduction of the vertical velocity fluctuations, (ii) Through the zero stress condition at the free surface that influences the diffusion of momentum, and (iii) through the boundary condition for the scalar. A two-layer structure develops for the turbulent diffusion of momentum, and a similar for the turbulent mixing of the scalar. We will present a imilarity theory for the two-layer structure which fits well results from direct numerical simulations and shows the influence of momentum diffusion on the diffusion of the scalar. Scaling laws for the thickness of the layers are derived based on the theory.

STRATIFIED BOUNDARY LAYER FLOW OF A GAS STREAM AND A LIQUID FILM PAST SOLID SURFACES

N. A. PELEKASIS, D. N. SMYRNAIOS, J. A. TSAMOPOULOS

Laboratory of Computational Fluid Dynamics, Department of Chemical Engineering
University of Patras, Greece

The steady two-dimensional laminar flow of an air stream, flowing past a solid surface at high Reynolds number, is examined in the presence of rainfall. As raindrops sediment on the surface they coalesce and form a continuous water film that flows due to shear, pressure-drop and gravity, in general. In the limit as the boundary layer and film thickness remain smaller than the radius of curvature of the surface a simplified lubrication-type formulation describes the flow field in the film, whereas the usual boundary layer formulation is applied in the gas phase. In the case of a flat plate and close to the leading edge, $x \to 0$, a piecewise self-similar solution is obtained, according to which creeping flow conditions prevail in the film whose thickness grows like $x^{3/4}$, whereas the Blasius solution is recovered in the air stream. Numerical solution of the governing equations in the two phases and for the entire range of distances from the leading edge, $x=O(1)$, shows that, in the case of flow past a NACA-0008 airfoil at zero angle of attack, a Goldstein singularity may appear far downstream on the airfoil surface due to adverse pressure gradients indicating flow reversal and eddy formation inside the liquid film and, possibly, flow separation. In addition it was found that there exists a critical water film thickness beyond which the film has a lubricating effect decelerating the appearance of singularity. Below this threshold the presence of the liquid film actually enhances the formation of singularity[1].

Local linear stability analysis is also performed for flow past a flat plate, assuming nearly parallel base flow in the two streams, and operating in the triple-deck regime. Two distinct families of eigenvalues are identified, one corresponding to the well known Tollmien-Schlichting (TS) waves that originate in the gas stream, and the other corresponding to an interfacial instability. It is shown that, for the air-water system, the (TS) waves are convectively unstable whereas the interfacial waves exhibit a pocket of absolute instability, in the streamwise location of the applied disturbance. Moreover, it is found that increasing the inverse Froude number (Fr^{-1}), indicating the increasing effect of gravity compared to inertia, results in shrinking the pocket of absolute instability until a critical value is reached, $Fr^{-1} \approx Fr_c^{-1}$, beyond which the family of interfacial waves becomes convectively unstable. In this context, increasing the rainfall rate or the free stream velocity results in extending the region of absolute instability over most of the airfoil surface[2]. Owing to this behavior it is conjectured that a global mode may arise at the interface that is responsible for most of the dynamic phenomena associated with the effect of rainfall. The nonlinear version of the triple-deck equations is currently under numerical investigation in order to verify the existence of a global mode and capture the evolution of unstable wave-packets in space and time for the case of large disturbances.

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FLUID MECHANICS AND RHEOLOGY RESEARCH OPPORTUNITIES IN PHARMACEUTICAL R&D TECHNOLOGIES

S. KIM

Parke-Davis Company, USA

Thanks to the recent completion of the human genome sequencing project (as well as advances in automation technologies for combinatorial chemistry), a new paradigm is emerging in pharmaceutical R&D. A new profile of the R&D pipeline is taking shape, based on the concept of massively parallel operations in discovery research (target discovery and development, high throughput screening and lead optimization). Fluid mechanics and rheology, as fundamental disciplines, are playing pervasive and enabling roles in pharmaceutical R&D technologies.

MODELS FOR FLOW OF NON-NEWTONIAN FLUIDS THROUGH POROUS MEDIA

J R A PEARSON

Schlumberger Cambridge Research & BP Instititute, University of Cambridge

The purpose of the ideas and models developed here is to enable flow-rate and dispersion predictions to be made when complex fluids are driven through porous media, typically rocks, by pressure gradients.

The role of meso-scale micro-models of a porous medium in developing continuum macro-models for Darcy-scale flow will be analysed. This will be based on existing averaging and homogenising techniques. Particular examples of capillary networks will be considered as suitable candidates. Approximate calculation methods for predicting flow and dispersion behaviour through these networks will be described. Methods for incorporating the time dependence and elasticity of thixotropic and elastico-viscous fluids into continuum formulations will be presented. Proposals for selecting and inverting laboratory-scale measurements on cores or packed beds of sand to yield suitable meso-scale model parameters will be put forward.

Potential applications will be described briefly.

A SUSPENSION MODEL FOR POLYMER SOLIDIFICATION RHEOLOGY

ROGER I. TANNER

School of Aerospace, Mechanical and Mechatronic Engineering, University of Sydney, Sydney, 2006, Australia

The events during solidification of flowing polymers are extremely complex, often involving partial crystallization. Many processes certainly need consideration of viscoelastic effects, and we present here a new, but elementary, model of solidification rheology based on suspension theory.

VISCOELASTIC CONTRACTION FLOWS: COMPARISON OF AXISYMMETRIC AND PLANAR CONFIGURATIONS

S. NIGEN, K. WALTERS*

Department of Mathematics, University of Wales, Aberystwyth, UK

Attention is given to experimental flows through contractions, with particular reference to the phenomenon of vortex enhancement. Two types of non-Newtonian elastic liquids are considered, namely constant-viscosity Boger liquids and also shear thinning liquids. A particular issue of interest is the differences observed between flow in an axisymmetric contraction and the corresponding flow in a planar contraction.

Provocatively, it is found that, whereas Boger liquids exhibit vortex enhancement in axisymmetric contractions, it is *absent* for these liquids in planar contractions. In contrasts, shear thinning elastic liquids show vortex enhancement in both axisymmetric and planar contractions.

We attempt to provide a comprehensive portfolio of behaviour in geometries with different contraction ratios and for different flow rates. It is our hope that the data will provide a challenge to the many workers in the field of computational rheology. Some consideration is also paid to the interpretation of contraction flow data in terms of “extensional viscosity”. We raise the obvious question as to whether the provocative differences between the behaviours of constant-viscosity and shear-thinning liquids reflect differences in uniaxial and planar extensional-viscosity levels.

VISCOPLASTIC BOUNDARY LAYERS

J-M. PIAU

Laboratoire de Rhéologie, BP 53
38041 GRENOBLE Cedex 9 – France

When a viscoplastic constitutive behaviour is assumed, well-known hypotheses and results obtained for viscous fluids have to be carefully re-examined. Very few studies considered the flow of viscoplastic fluids along a wall.

Oldroyd [1947] suggested a particular similarity solution for the plastic boundary layer created by a knife entering slowly a Bingham type material. *Acrivos* [1960] extended the natural convection boundary layer theory to a viscous power law type material.

Both models considered are particular cases of the Herschel-Bulkley model, the flow equations of which in a long domain have been studied by *Piau* [1996].

Paying particular attention to normalizing pressure terms, theoretical results are obtained for viscoplastic Herschel-Bulkley boundary layers. They are compared both to previously published solutions and to new experimental data.

CONVERGENCE OF A REGULARIZATION METHOD FOR FLOW OF A BINGHAM MATERIAL PAST A SPHERE

BENJAMIN T. LIU[1], SUSAN J. MULLER[1], MORTON M. DENN[2]

[1] Lawrence Berkeley National Laboratory and Department of Chemical Engineering,
University of California, Berkeley, CA 94720-1462 USA
[2] Benjamin Levich Institute for Physico-Chemical Hydrodynamics,
City College of CUNY, New York, NY 10031 USA

The development and location of yield surfaces in non-viscometric flows of Bingham materials has long been a subject of controversy because of the difficulty of carrying out reliable computations for the exact Bingham model. We have used a regularization method to study creeping flow of a Bingham material past a solid sphere; convergence to the exact Bingham model can be established for appropriate limiting behavior of the second invariant of the deformation rate tensor and the product of this invariant with the square of the regularization parameter. The drag coefficient and streamlines approach limiting values with increasing values of the regularization parameter; the location of the yield surface in the far field continues to move to greater distances from the sphere surface with increasing regularization parameter, however, until a value of the regularization parameter is reached at which rounding and truncation errors preclude reliable calculations. It appears that a limiting yield surface can nevertheless be estimated from the sequence of differences in the strain-rate fields for successive values of the regularization parameter. This yielded region is significantly larger than that reported in prior studies. Unyielded equatorial and polar regions computed close to the sphere for small values of the regularization parameter reduce to points with the approach to Bingham behavior.

PARTICLE MIGRATION AND SEGREGATION IN SUSPENSION FLOWS UNDERGOING SHEAR

ANDREAS ACRIVOS

For the best part of the last century, it has been taken for granted that concentrated suspensions of non-colloidal particles can be modeled as effective Newtonian fluids having an effective relative viscosity which is uniquely determined by the local particle volume fraction. Experiments over the past twenty-five years have demonstrated, however, that the rheology of such suspensions often differs in a fundamental way from that of a Newtonian fluid of comparable viscosity. This is due to the action of shear-induced particle diffusions from regions of high shear to low and from regions of high concentration to low which can generate a non-uniform concentration profile within the sample being sheared even under creeping flow conditions. Consequently, when a well-mixed suspension of neutrally buoyant particles is made to flow in a long tube or channel, a fully developed particle concentration profile is attained in which the concentration increases monotonically from the wall to the center. The effective viscosity of the suspension adjacent to the wall is thereby reduced and hence, for a given volumetric flow rate, the pressure drop in such a system is significantly lower than if the particles were uniformly distributed. Shear-induced diffusion is also responsible for the phenomenon of viscous re-suspension whereby an initially settled bed of heavy particles in contact with a clear fluid above it can re-suspend under the action of shear. These and other examples will be presented as well as the mathematical models that have been developed successfully to describe the experimental findings.

Nevertheless, during the past couple of years, a number of experimental observations have been made of particle segregation in a partially filled horizontal Couette device and a rotating cylinder which remain totally unexplained.

ORAL CONTRIBUTIONS

RHEOLOGY OF DENDRIMERS AND THEIR HYBRID COPOLYMERS WITH LINEAR POLYMERS

MICHAEL E. MACKAY[1], MIYOUN JEONG[1], R. VESTBERG[2], C.J. HAWKER[2]

[1]Dept. of Chemical, Biochemical and Materials Engineering
Stevens Institute of Technology
Castle Point on the Hudson
Hoboken, N.J., 07030
[2]IBM Almaden Research Center
650 Harry Road
San Jose, CA, 95120

We have found that dendrimers show little evidence of entanglements even up to molecular masses near 100 kDa. The rheological properties of linear-dendrimer hybrid block copolymers have recently been measured to determine if this unique behaviour extends to this class of polymers.

Indeed it appears as if the dendrimer architecture does make a difference in the rheological properties, even when the molecular mass of the linear block is quite large, by showing a viscosity decrease. However, the amount of decrease can be modified depending on the thermal and thermodynamic history of the block copolymer. We believe the dendrimer acts as a nanoscopic object which can significantly alter the thermodyamic and rheological state of the system that linear polymers can not accomplish.

COMBINING NMR AND CLASSICAL RHEOMETRY TO EVALUATE THE VISCOELASTIC PROPERTIES OF MAIN-CHAIN NEMATIC LC POLYMERS

A. VÉRON, A. F. MARTINS

Dept. Ciência dos Materiais, Faculdade de Ciências e Tecnologia,
Universidade Nova de Lisboa, 2825-114 Caparica, Portugal

The rheological behaviour of main-chain nematic liquid crystalline polymers in steady shear flow is analysed by combining NMR experimental data with theoretical predictions of Martins' constitutive equations. This theory provides simple analytical expressions for the nematic flow functions. They are related to the Leslie viscosities and two structural parameters (a relaxation time τ, and a parameter $-1 \leq \varepsilon \leq 1$ characterising the non-affinity of the polymer response). In recent years, measurements of four out of the five viscosity coefficients, namely α_1, α_2, α_3, $\alpha_4+\alpha_5$, by Rheo-NMR techniques, have been reported in literature for several nematic polymers. In such cases, when classical rheometry data are also available, it is of interest to calculate the flow functions from the experimental Leslie viscosities and to compare the results with the rheometry data. In the case of PBLG the two normal stress differences are known, the fifth viscosity and the two structural parameters have been determined. In cases where only the first normal stress difference is known, the fifth viscosity and the relaxation time may be evaluated assuming a reasonable value for ε. When no rheological data is available, the main qualitative features of normal stress differences may be predicted from the NMR data and an estimate of α_5 based on theoretical arguments supported by the theory of Doi.

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MICROEMULSIONS OF ABA AMPHIPHILIC BLOCK COPOLYMERS AND SURFACTANTS

LIORA BRAUN-SHMUELI, ORTAL NETANEL, OREN REGEV, MOSHE GOTTLIEB

Chemical Engineering Department, Ben Gurion University, Beer Sheva 84105, Israel

The system composed of oil (decane), water and an ABA amphiphilic block copolymer is capable of exhibiting an extremely rich phase and rheological behavior. In this paper we describe the rheological properties of a synthetic amphiphilic block copolymer dissolved in a water-in-oil microemulsion with and without the stabilizing effect of small molecular weight surfactant molecules. The block copolymer is an ABA type copolymer composed of poly(oxyethylene) (PEO) as the hydrophilic A block and poly(dimethyl siloxane) (PDMS) as the hydrophobic center B block.

The resulting copolymer is insoluble in water and hardly soluble in decane (good solvent for the PDMS). In the presence of water in oil microemulsion stabilized by the small molecular weight surfactant AOT a one-phase region is maintained when the copolymer is added. Yet, peculiar rheological behavior is observed. For constant water-microemulsion concentration (ϕ) addition of polymer increases the system viscosity as expected. Yet, the lower ϕ the higher the viscosity and at high ϕ the effect of polymer addition is quite low. Furthermore, the insoluble block copolymer in oil turns into a gel-like one phase system upon addition of small amounts of either water or water and surfactant solution. Experiments show that a maximum in elasticity or viscosity is attained at a droplet concentration equivalent to about 80 polymer chains per drop. Small angle x-ray and neutron scattering experiments were carried out to elucidate the system morphology.

HIGH FREQUENCY DYNAMICAL VISCOMETRY ON CONFINED EMULSIONS

A. ROMOSCANU, M.B. SAYIR, K. HÄUSLER[1], I. ROBERTS[2]

[1]Swiss Federal Institute of Technology, Zurich, Switzerland.
[2]Nestlé Research Center, Lausanne, Switzerland.

A high frequency shear rheometer was designed on the principle of a translational oscillator carrying out forced vibrations in the vicinity of one of its resonance frequencies. The phase angle between the applied torque and the measured response is fixed by controlling and stabilising the frequency continuously with the help of a phase-locked loop. By using a specially gated electronic circuit, the same electromagnetic transducer can be used for both driving and sensing. The increase in damping resulting from the contact with the fluid, i.e. its oscillatory shearing, is deduced from the increase in the frequency difference for a given phase difference. Since the phase-locked loop stabilises the frequency within 0.001 Hz, the accuracy of the measurement is very high, especially if the temperature is maintained sufficiently constant. The simplicity and robustness of the vibrational rheometer as well as its insensitivity to external vibrations and disturbances qualify it for in-line measurements, as well as for high-frequency measurements (typically 0.5 – 10 kHz), a frequency range which is out of reach for conventional rheometers.

Because of the viscous dissipation and the relatively high frequency, the penetration depth of the shear disturbance in a half-space filled with the fluid is relatively low (a typical value in water is 15 μm at a frequency of 1 kHz), i.e. only local rheological characteristics in a boundary layer in the vicinity of the tangentially oscillating body are measured. For fluids which are heterogeneous on a scale which is similar to the sheared layer thickness, like emulsions or suspensions, concentration gradients occurring in this layer have to be controlled, for the parameters measured by the high frequency probe reflect these local, concentration dependent properties.

In the present paper, results obtained with a probe designed to measure films of variable but controlled thickness are presented. An important feature of the thin film probe is that the gap width can be set to be smaller than the penetration depth of the viscous disturbance in a half-space, thus forcing the whole sample to be sheared. The influence of various factors like emulsion volume fraction, particle size distribution and interfacial tension on the probe damping is measured. Further, the dynamic deformational behaviour of dispersed phase droplets in a oscillatory shear flow of small amplitude is observed with the help of a high speed camera.

In this work, we also look at homogeneous fluids, for which an analytical approach is preferred. With the help of a theoretical modelling of the oscillating flow of the fluid confined in the gap, the relevant rheological parameters of the fluid are linked to the increase of the damping and to the measured resonance frequency shift. For our analytical approach, we consider various rheological models for the fluid, among which Newtonian and shear thinning (power-law) ones.

TELECHELIC POLYELECTROLYTES: NEW DEVELOPMENTS IN THE RHEOLOGY OF AQUEOUS FORMULATIONS

CONSTANTINOS TSITSILIANIS

Department of Chemical Engineering, University of Patras, 26500 Patras Greece
and Institute of Chemical Engineering and High-Temperature Chemical Processes,
ICE/HT-FORTH, P.O.Box 1414, 26500 Patras, Greece

Model associative polymers constituted from a long polyelectrolyte end-capped with short hydrophobic polymeric blocks were synthesized by “living” polymerization methods and their behavior were explored in aqueous media. These kind of systems exhibit some unique rheological properties compared to those obtained from the classical non ionic associative telechelic polymers (e.g. end-capped poly(ethylene oxide). Physical gels are formed in dilute solutions, characterized by low gel concentrations, yield stress, complex steady shear viscosity profile, high plateau modules and long relaxation times. These properties are attributed to the formation of a transient network constituted from hydrophobic physical crosslinks interconnected by stretched polyelectrolyte chains. The influence of several factors, such as polymer architecture (ABA, ABC, 3 armed star), nature and length of the end-blocks, degree of neutralization of polylectrolyte e.t.c., on the rheological properties were investigated. ABC types seem to be the most promising associative polymers for applications as strong thickeners in aqueous formulations.

VISCOELASTICITY AND NETWORK STRUCTURE OF WATER-BASED POLYSACCHARIDE SYSTEMS

ANDREJA ZUPANČIČ, URSKA FLORJANČIČ, MIHA ŽUMER

University of Ljubljana, Faculty of Chemistry and Chemical Technology, Department of Chemical Technology,
Chair of Chemical, Biochemical and Ecological Engineering, Aškerčeva 5, SI-1000 Ljubljana, Slovenia
phone:+386 1 476 04 15, fax: +386 1 426 45 77

The flow behaviour and the viscoelastic properties of polysaccharide systems: welan, xanthan, gellan, and carboxymethyl cellulose, have been systematically examined at low polymer concentrations in a wide range of mutual ratios of studied polymers. Pure polymer samples were prepared by dissolving the powdered polymer in distilled water at ambient temperature during mechanical stirring. Before the rheological tests, samples were stored for two days to ensure a complete wetting of the polymer. The systems composed of two polysaccharides were prepared at the same concentration by blending pure water-based polymer samples.

The rheological tests were performed at 20°C under steady and oscillatory shear conditions using the controlled stress rheometer HAAKE RheoStress RS 150, equipped with cone/plate and double cone sensor systems. The analysis of viscoelastic data under non-destructive shear conditions was performed by using different models for describing the mechanical spectra in linear viscoelastic regime.

At the same polymer concentration pure water-based samples exhibited different type of rheological behaviour, from polymer solution to weak gel. A wide range of rheological properties can be achieved by varying polymer concentration and by preparing different mixtures of polymers at various mutual ratios. Among different aqueous polymer mixtures two combinations of polysaccharides were selected: one of them enabled us to follow the transition from polymer solution to weak gel behaviour, the other showed a synergistic effect between weak gel and polymer dispersion. Further attention was focussed on the investigation of rheological behaviour of selected polysaccharide mixtures at different polymer concentration.

Due to different temperature dependencies of pure water-based polymer samples, the effect of temperature on the rheological properties of polysaccharide mixtures requires further investigations.

Aim of our work is to examine a proper non-Newtonian fluid for further research of mixing process in laminar flow regime. The mixing of non-Newtonian fluids is one of the most complex processes to understand. The industrial fluids often exhibit complex rheological behaviour, and their viscoelastic properties significantly influence the mixing process. This work presents the results of detailed rheological investigation of weakly structured materials with suitable viscoelastic properties for mixing operation under the conditions of laminar flow. Knowledge of structural conditions in weakly structured hydrophilic polymers and detailed description of rheological behaviour can help us to understand the flow patterns in mixing processes.

Key words: rheology, viscoelasticity, polysaccharides, weak gels

ELONGATIONAL RHEOLOGY OF BRANCHED POLYPROPYLENE

A.D. GOTSIS

Dept. of Polymer Materials and Engineering, Faculty of Applied Sciences, Delft University of Technology
Julianalaan 136, 2628 BL Delft, the Netherlands

Conventional polypropylene made by Ziegler-Natta or metallocene catalysis consists of highly linear molecules with narrow molecular weight distribution. As such, it can not be readily used in processes where substantial extensional flows may occur, e.g. in foaming, thermoforming or film blowing. This is caused by the low melt strength of polypropylene and the lack of strain hardening of its elongational viscosity. The melt strength of linear polypropylene (PP) can be enhanced by the presence of long chain branches. In this work such branches were added to a linear PP by means of reactive extrusion in the presence of selected peroxy-dicarbonates [1,2]. This method has been found to result in the addition of low numbers of long branches, which can be measured by SEC in combination with on-line viscosity measurements of the fractions [3]. The branches, however, are added at the high molecular weight chains and this modification was found be adequate to improve the melt strength of PP considerably. The Melt Flow Index (MFI) increased slightly. The extrudate swell and the elasticity (G') of the samples also increased. The zero shear viscosity increased with the degree of branching, while the viscosity at high shear rates of all samples remained the same. It seems that the use of peroxy-dicarbonates in the extruder is an economic alternative to the electron beam irradiation techniques that are used to produce highly branched commercial polypropylene. Even though the Rheotens measurements established the differences in melt strength between the several materials, they were less sensitive in distinguishing the extent of branching than the extensional rheology, which remains an excellent probe for the molecular structure of polymers. The values of the stress at the time of break of the filament and the relative degree of strain hardening, on the other hand, can show significant differences between the effectiveness of the modifications. The use of peroxy-dicarbonates to modify PP resulted in distinct strain hardening of the elongational viscosity. The theory of rubber elasticity was used to relate the degree of strain hardening to the degree of branching. We also studied the influence of the structure of the peroxy-dicarbonates used for the modification on effectiveness of the modification and the extensional properties of the resulting material. It was found that peroxy-dicarbonates with larger alkyl groups were more efficient and resulted in PP with the most branches and the highest elasticity.

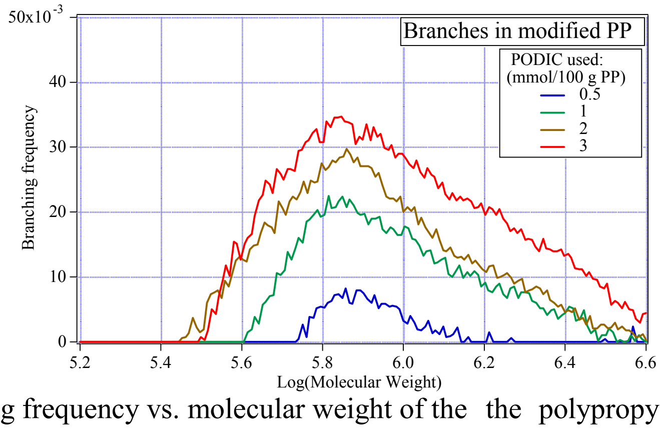

Fig. 1: Branching frequency vs. molecular weight of the the polypropylenes modified with increasing amount of peroxy-dicarbonates

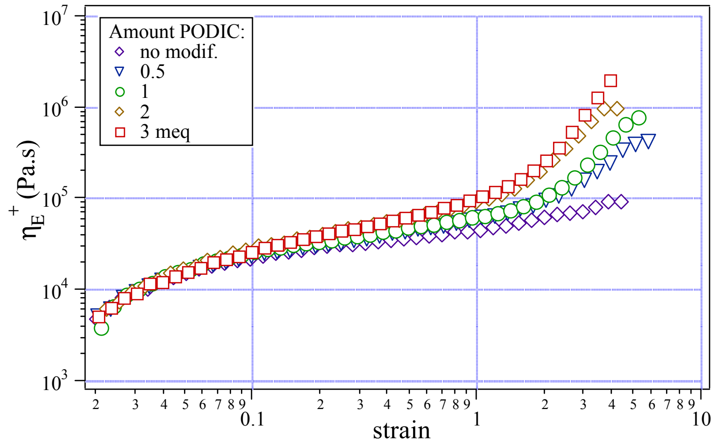

Fig. 2. Growth of the elongational viscosity of modified polypropylene samples (at a str. rate of ~0.1 s^{-1})

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RELAXATION MECHANISMS IN HYPERSTAR MELTS

D. VLASSOPOULOS (1), T. PAKULA (2)

(1) FO.R.T.H., Institute of Electronic Structure and Laser, Box 1527,71110 Heraklion, Crete, Greece
(2) Max-Planck Institut fuer Polymerforschung, Postfach 3148, D-55021 Mainz, Germany

We investigate the relaxation of complex macromolecular objects representing model branched polymers. They include multiarm stars, dense combs and aggregates formed from end-functionalized linear and star polymers. These systems have been synthesized anionically, yielding well defined polymers and architectures (Roovers, Hadjichristidis). The relaxation processes, extracted from linear rheological measurements are rationalized based on parallel structural studies using SAXS, theoretical support from molecular theories on star polymers using the tube model, and computer simulations. Using a generalized isofrictional plot of relaxation times versus molecular weight, we present the features of relaxation of branched polymers that are universal, and discuss the additional relaxation modes and relevant complications arising from the topology of the examined systems.

POLYMER BRUSHES UNDER STRONG SHEAR FLOW IN A GOOD SOLVENT

**C. TOPRAKCIOGLU¶, D. ANASTASSOPOULOS¶, A. VRADIS¶,
A. PAPAYIANOPOULOS¶, S. BAKER§, A. MENELLE┼**

¶ Department of Physics, University of Patras, Patras, Greece.
§ Harvey Mudd College, Claremont, California, USA.
┼ Laboratoire Leon Brillouin, C.E –Saclay, France

Recent theoretical calculations on the behavior of polymer brushes in strong shear flow regimes have produced mixed predictions. The brush height (i.e. the layer thickness of the brush) is expected to increase by some theories, while others find it should remain unchanged or even decrease under shear flow. We have used neutron reflectivity techniques to prove directly the volume fraction profiles of polystyrene brushes under strong shear flow in toluene (a good solvent) at shear rates ranging from ca. 10000 to ca 20000 reciprocal seconds. We find that the brush profile remains unchanged up to 1x 10^4 s^{-1}, but at shear rates in the region of ca. 1.5x10^4 s^{-1} desorption of the chains emerges abruptly. This result is in broad agreement with the dual-chain model of Aubouy, Harden and Gates (Journal de Physique II 1996, 6, 969). We have currently extended our investigation to “mixed” brushes (i.e. polymer brushes consisting of chains with two different molecular weights) where the brushes structure is expected to be more susceptible to shear flow.

BLOCK COPOLYMERS AS EMULSIFIERS IN HOMOPOLYMER BLENDS: EFFECTS OF ADDITIVE MW, ARCHITECTURE, AND COMPOSITION[#]

SPIROS H. ANASTASIADIS[*], HARIS RETSOS

Foundation for Research and Technology – Hellas, Institute of Electronic Structure and Laser
P. O. Box 1527, 711 10 Heraklion Crete, Greece
and
University of Crete, Physics Department
P. O. Box 2208, 710 03 Heraklion Crete, Greece

The effect of the addition of block copolymers on the reduction of the interfacial tension between two immiscible homopolymers is investigated as a function of the additive concentration, molecular weight, macromolecular architecture, and composition for polystyrene / polyisoprene blends in the presence of polystyrene - polyisoprene block and graft copolymers. The interfacial tension reduction is a non-monotonic function of the copolymer molecular weight at constant copolymer concentration. As the additive molecular weight increases the interfacial tension reduction, $|\Delta\gamma|$, goes through a maximum. This is related with the increased tendency of micelle formation for high copolymer molecular weights, which is verified by small-angle X-ray scattering. The results are discussed in relation to theoretical predictions for polymer / polymer / copolymer mixtures. At the same time, the reduction is a strong function of the additive architecture with graft copolymers leading to a larger reduction; for graft copolymers, the maximum efficiency observed was for a non-symmetric copolymer composition. The results strongly indicate the importance of micelle formation on the efficiency of block copolymers as emulsifying agents.

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THEORETICAL AND EXPERIMENTAL INVESTIGATION OF NON-LINEAR VISCOELASTIC AND VISCOPLASTIC RESPONSE OF AMORPHOUS POLYMERS

E. KONTOY, G. SPATHIS

Department of Applied Mathematical and Physical Sciences,
Section of Mechanics, National Technical University of Athens
5 Heroes of Polytechnion, GR-15773, Athens , Greece

The prediction of the inelastic mechanical behavior of glassy polymers in terms of monotonic loading, creep and relaxation is of great importance. However, these aspects of deformation behavior usually are treated separately. In this work, the non-linear viscoelastic and viscoplastic response of glassy state is predicted in terms of a unified model. This model treats the initial stages of deformation up to the yielding, as a thermally activated process, while the subsequent plastic path is quantitatively described through a mechanism based on the distributed nature of strain around specific regions with high free volume. The elastic energy stored in these regions attains a critical value, leading to the transition of these regions into a non-recoverable state, exhibited macroscopically by plastic deformation. It was suggested that the deformation mechanism is the same under a constant crosshead speed experiment, as well as in a creep test with varying stress levels over a wide range. Tensile and compressive creep experiments were conducted for polycarbonate at room temperature, at various stress levels, while the deformation could be measured very accurately at every localized region along the total gauge length. The experimental procedure followed is based on a non-contact method with a laserextensometer technique.

The material properties required in the model, and related to thermal activation, were obtained from creep experiments, in terms of creep strain rate versus strain. Moreover, two internal variables, describing the distribution of strain, namely the yield strain (mean value of the probability density) and the standard deviation were also needed for the model prediction of plastic strain rate.

The model hereafter, will be proved to be capable of predicting the nonlinear viscoelastic – viscoplastic response under a nonmonotonic loading test for various crosshead speeds test , as well as the creep strain versus time for various stress levels.

DETERMINATION OF THE RHEOLOGICAL PROPERTIES OF MICROCAPSULES

M. CARIN[1], C. POSTEL[1], M. RACHIK[2], D. BARTHÈS-BIESEL[1]

1- UMR CNRS 6600, UTC, BP 20529, 60205 Compiègne, France
2- Laboratoire Roberval, UTC, BP 20529, 60205 Compiègne, France

Microcapsules are fluid-filled cells with thin membrane walls which are now used in a wide range of industries (pharmaceutic, agriculture, food, cosmetic, biotechnology). The rheological properties of artificial capsules play an important role in determining their suitability for specific applications. However, the mechanical properties of the capsule membrane are rarely known with precision because they are quite difficult to measure. An experimental technique commonly used for the measurement of the bursting force of the membrane consists in squeezing the capsule between two parallel plates. However the squeezing force is a non linear function of the distance between the plates. It depends on the initial geometry of the capsule and on the membrane properties.

The experimental set-up allows a continuous visualization of the capsule deformed shape with two video-cameras giving side and bottom views (Figure 1). The edge of the membrane, the surface and the volume of the capsule are determined by means of image analysis. Loading-unloading and stress relaxation experiments are performed on capsules with different membranes (alginate and protein or polyamide).

In order to analyze the experimental data in terms of the membrane mechanical properties, a model of the compression process is designed. A finite element computation of the large deformations of an axisymmetric membrane containing an incompressible material is done. Different models of the membrane are compared (2D thin shell with or without bending rigidity, 3D homogeneous solid).

The membrane behaviour is described by a rubber-like constitutive law. The rheological constants are identified by an inverse method from the experimental data. To validate the approach, various simulations are performed and the numerical results are compared with experiments (Figures 2 and 3).

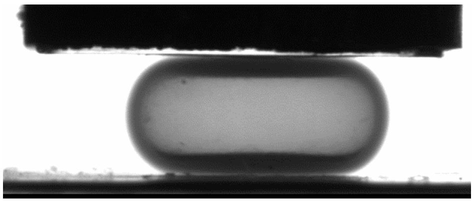

Fig. 1: Side view of the deformed capsule

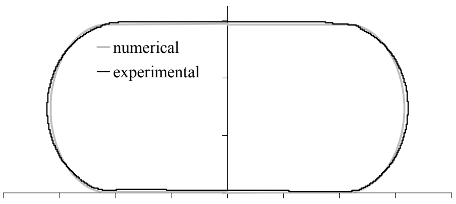

Fig. 2: Comparison of the predicted and experimental profiles

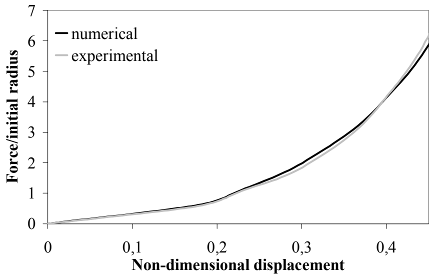

Fig. 3: Comparison of the predicted and experimental loading curves

THE INFLUENCE OF WALLS ON PARTICLE MIGRATION IN SUSPENSIONS

WENXIAN LIN*, ALLEN KAISER*, ALAN L. GRAHAM*, MARC S. INGBER**

*Texas Tech University
**University of New Mexico

The trajectories of particles subjected to inhomogeneous shear flows are affected by the presence of containing walls. In this coupled experimental and numerical effort, particles subjected to a number of different inhomogeneous shear flows are observed to migrate away from the containing walls. Experiments on suspensions of neutrally buoyant spheres in Newtonian fluids reveal that clusters of particles placed near the containing walls of a wide-gap Couette migrate towards the center portion of the gap, but the migration rates that are dependent on the local shear rate gradients. Falling-ball experiments in suspensions of similarly sized neutrally buoyant spheres in which a dense ball is allowed to settle near a containing wall show that the falling ball experiences a lateral migration away from the containing walls. The extent of this migration increases as the distance to the wall decreases and the particle concentration increases. Fully three-dimensional boundary element simulations confirm these experimental observations and show the effect on suspensions subjected to identical shear rate gradients in the proximity of walls and in flow fields without bounding surfaces.

DYNAMICS OF DEFORMABLE SURFACTANT-COVERED DROPS

PETIA VLAHOVSKA, JERZY BLAWZDZIEWICZ, MICHAEL LOEWENBERG

Department of Chemical Engineering, Yale University, P.O.Box 208286, New Haven CT 06520-8286, USA

Complex fluids have rich rheological behavior that stems from relaxation of the material microstructure. Predicting the rheology and other macroscopic properties of these systems relies on a detailed understanding of the particle-level microhydrodynamics.

We study the effect of insoluble surfactant on deformation of a spherical drop in shear and extensional flows at low Reynolds number. A second order perturbation analysis and numerical simulations have been developed for the evolution of the drop shape and surfactant distribution. A linear equation of state relating interfacial tension to the local surfactant concentration is considered. Surface diffusion and viscosity effects are neglected. Analytical results are obtained for the small-capillary-number (weak flow) and high-drop-viscosity regimes. The expansions converge over a wide range of parameters; the second order weak-flow expansion predicts drop deformation in extensional flow up to the critical capillary number. Three-dimensional boundary integral simulations are used to explore drop dynamics under large deformation conditions. Adaptive restructuring of the computational grid allows resolution of high curvature regions and strongly deformed surfactant distributions.

Our analytical and numerical results indicate that under identical conditions (i.e. average surface tension, shear rate), surface tension variations, originating from surfactant redistribution, enhance drop deformation. Drop deformation decreases with surfactant layer elasticity in strong flows but under weak flow conditions the drop shape is insensitive to the elasticity.

The one-drop contribution to the stress of a diluted emulsion of deformable surfactant-covered drops is calculated. The results reveal non-Newtonian rheology with shear thinning viscosity and nonzero normal stresses. The shear viscosity at low shear rates is given by the value for suspension of rigid spheres and, for low surfactant layer elasticity, decreases to the value for emulsion of drops with a surfactant-free interface. Our second-order theory describes quantitatively the shear thinning and normal stresses obtained by our numerical simulations.

This work provides a quantitative basis for predicting drop deformation and the rheology of emulsions. Moreover, it can give useful insights for understanding the behavior of other complex fluids with similar microstructure such as polymer blends, biological fluids, etc.

EFFECTS OF TURBULENT MOTION ON BREAKDOWN PROCESSES OF NATURAL FIBERS

PAOLO PERONA, SEBASTIANO SORDO

Dipartimento di Idraulica, Trasporti e Infrastrutture Civili Politecnico di Torino
Corso Duca degli Abruzzi, 24 – 10129 Torino (ITALY)

In this work some first results concerning the effects of turbulent motion on the breakdown processes occurring on diluted apple, peach and pear purees, are presented. These fruits have a different internal structure, typically associable to an agglomerate of coiled filament-like particles (apple puree) or to an ensemble of irregular spherical-like particles (peach puree) or either ones (pear puree) scattered within a main heterogeneous liquid phase. These results can be of interest for two reasons: firstly, the fluid dynamics behavior of the diluted products seems to show some evident influence of the dispersed solid phase (i.e. solid fibers) within the liquid phase (i.e. the whole liquid matrix) different from one product to another. Secondly, industrial processes must take in account the possibility that turbulent motion, often arising in diluted fruit purees, can seriously damage the internal structure of the fluid causing variations on the rheological and physicochemical properties. In order to investigate such effects, an experimental setup based on the rectilinear pipe viscometer principle was used to measure differential pressures Δp over a length L and flow rate Q, at different pulp concentration. In order to classify the basic fluid dynamic behavior, a preliminary rheological investigation was done for all the analyzed products. Since the breakdown processes occur whether in laminar or in turbulent motion, it is very important to consider their effect already during the rheological characterization. For laminar motion we found that this effect was relevant only for non-diluted apple puree and this permitted to consider the diluted products as time independent behavior fluids, generally well described at high shear rates as a power law model. At a given dilution level, transition to turbulence occurred and the corresponding resistance laws were searched by means of the Dodge and Metzner method (1959), by the which one could well predict the behavior of peach and pear diluted purees. Conversely, for the case of diluted apple puree, the experimental data did not follow the empirical law predicted by the method. This behavior lead us suppose it might be a consequence of the different internal structure of products. Since apple puree seems to be quite sensitive to the breakdown processes, a first hypothesis was related to the possibility that as more mechanical stresses rapidly increase – being mainly influenced by the velocity turbulent components – the more the processes of breaking of the internal structure are emphasized. In this case experimental data measured within the turbulent regime would not be reliable because they are related to rheological properties that do continuously vary during the experimental condition. As a consequence the measured curve lies on different curves at different breakdown structure degree. In order to verify the hypothesis two equal volume samples of diluted apple puree, one in laminar motion and the other in turbulent motion, were forced to circulate in a loop until the breakdown process was complete. A successive rheological characterization evidenced the effects induced by the turbulent motion, different from those induced by the laminar one. A further photographic investigation realized on the two samples by means of an optics microscope, confirmed that additional kinetic energy typical of the turbulent regime could be considered responsible of the fractured aspect of the fibers. Resistance law for the sample that had suffered breakdown process in laminar flow condition, do not reach – as the other purees – the corresponding empirical law. Conversely, resistance law of the sample having suffered breakdown process in turbulent flow conditions, clearly shows that experimental data are, now, closed to the empirical Dodge and Metzner law. Final observations are related to the fact that turbulence seems to have strong effects on the internal structure of apple puree, even when they are diluted, more than for other fruit purees. This effect clearly arises both on rheological parameters and at microscopic examination. The final interesting point is related to the fact that experimental data, after having reach the empirical law, still show a deviation from it. This behavior appears to be “curious” and seems to be imputable to a sort of drag reducing effect, also suggested by the actual un-coiled form of the solid fiber, spread within the liquid matrix.

THREE-LOBED SHAPE FORMATION OF CAPTIVE FERROFLUID DROPS

A. G. PAPATHANASIOU, A. G. BOUDOUVIS

Department of Chemical Engineering, National Technical University of Athens,
Zografou Campus, Athens 15780, Greece

Ferromagnetic liquid drops held in captivity between two horizontal plates suffer cross-sectional shape instabilities under the action of a vertical DC magnetic field of varying strength. The instabilities result from the competition between magnetic force, surface tension and gravity. In this work is reported the formation of stable, symmetric three-lobed equilibrium. Their connectivity with other four-lobed, asymmetric three-lobed and two-lobed shapes as magnetic field strength varies is studied experimentally. The symmetric three-lobed shapes are found to evolve into bended two-lobed ones by slowly decreasing the field strength; however, when the field strength increases, the reverse transition is not observed. Moreover, two-lobed shapes suffer a bending transition, by increasing the field strength, which is found to be hysteretic.

STATIC YIELD STRESS MEASUREMENTS OF SUSPENSIONS

D. DE KEE, L. ZHU, K. PAPADOPOULOS

Department of Chemical Engineering
Tulane University , New Orleans, LA 70118

We will discuss a new slotted-plate to directly measure static yield stresses of suspensions. Possible wall effects associated with our original yield-stress plate instrument] have been minimized. Yield-stress experiments were conducted on both high-concentration (TiO_2) and low-concentration (bentonite) aqueous suspensions. Our new setup avoids the disadvantages of the vane instrument, possible secondary flow between the blades as well as a non-uniform stress distribution along a virtual cylindrical surface. Yield stress values of TiO_2 suspensions were compared with the values obtained via a variety of other methods, including indirect extrapolation from steady-shear data, vane creep testing, and vane stress-ramp measurements using an SR-5000 rheometer. Very small yield stress (up to $\sim 10^{-4}$ Pa) measurements of low-concentration (2 wt.%) bentonite suspensions could be determined only with our slotted-plate device. The vane method could not measure yield stress values of bentonite suspensions of less than 7 wt. % concentration. Relaxation tests on high-concentration suspensions indicated that these suspensions may not be purely elastic below yield stress.We also plan to discuss results of a finite element analysis as well as results from measurements on silicon nitride mixtures.

VARIATIONAL INEQUALITIES IN VISCOPLASTIC FLUIDS - THEORY & APPLICATIONS

R. R. HUILGOL

School of Informatics and Engineering
Flinders University of South Australia
Adelaide, Australia

In the flows of viscoplastic fluids, it is shown that a bound on the rate of dissipation due to the yield stress can be used to obtain a stress power inequality, which applies to every flow of such a fluid. When this result is substituted into the equations of motion, one obtains a variational inequality which includes both the body force and acceleration terms; as far as the latter is concerned, both local and convected terms can be incorporated into the inequality.

After a brief discussion of the forms the inequality takes in many flows of interest, such as flow past a sphere, a sudden contraction/expansion flow, and free surface flows including viscometers, attention is focussed on flows in pipes of arbitrary cross-section. It is shown that if the pressure gradient falls below a critical value, the flow will come to rest in a finite amount of time. On the other hand, if the pressure gradient exceeds this critical value, then an upper bound on the steady flow rate can be obtained. These results, which are valid for all yield stress fluids, are simplified to those applicable to Bingham fluids, leading to explicit formulae involving the viscosity and the yield stress.

THE BEHAVIOR OF ELECTRORHEOLOGICAL FLUIDS IN TORTIONAL FLOW

BASIM ABU-JDAYIL[1], PETER O. BRUNN[2]

[1]Chemical Engineering Department
Jordan University of Science & Technology
P.O. Box: 3030, 22110 Irbid, JORDAN
[2]Department of Fluid Mechanics
University of Erlangen-Nurnberg
Gauerstr. 4, 91058 Enlangen, GERMANY

In this article, we report experiments on experimental and commercial electrorheological (ER) fluids in tortional flow. The electrorheological flow properties of ER-fluids were measured using a conventional rotational viscometer (a concentric-cylinders system). Then a torsional flow device (clutch) was designed and constructed. The flow curves measured with this device were compared with flow curves from the viscometer. The agreement between the two devices is encouraging. To study the influence of inhomogenous flow conditions besides the influence of the inhomogeneity of the electric field on the behavior of an ER-fluid in a clutch mechanism, oblique plates were used, where an oblique plate was fixed at the bottom plate of the clutch. The top plate was kept horizontal. Relative to the smooth plates, the improvement of the ER-effect corresponds to an average factor of 2.5 in the entire range of the measured field strength. This improvement in ER-effect seems be tied to the increase in local field strength at the thick rim of the oblique plate.

INFLUENCE OF MACROMOLECULAR ASSOCIATIONS ON THE DILUTE PROPERTIES OF A CLAY SUSPENSION

THIERRY AUBRY, FRÉDÉRIC BOSSARD, MICHEL MOAN

Laboratoire de Rhéologie, Université de Bretagne Occidentale
6, avenue Victor Le Gorgeu, 29285 Brest Cedex – France

In this work, a dilute Laponite suspension is studied in the presence of an associative polymer, namely hydrophobically associating (hydroxypropyl)guar, and its (non-associative) precursor. Using different investigation techniques, including sedimentation and viscometric measurements, evidence of the influence of the hydrophobic groups on the macroscopic properties of dilute Laponite suspensions is shown. Adsorption isotherms show that hydrophobic groups do not seem to have a major influence on the adsorption process : both polymers have nearly the same affinity to the clay surface, even though the amount of adsorbed modified macromolecules is somewhat higher than that of the non-modified ones at solid surface saturation. As far as the viscometric properties of the suspension are concerned, the main difference between the associative and the non-associative polymers appears at polymer concentrations above solid surface saturation. In this concentration range and at low shear rates, adding non-associating macromolecules is shown to lead to the formation of entities, whose relative contribution to flow resistance does not depend on the polymer concentration; whereas addition of associating macromolecules leads to the formation of entities, whose relative contribution depends strongly on the polymer concentration. Besides, on time scales lower than the average lifetime of the associating junctions, the relative contribution of both polymers to the viscous behavior of the suspension is quite similar and does not depend on the polymer concentration. The sedimentation and viscometric results of this comparative study are discussed in terms of polymer/clay interactions, focussing on intermolecular associations between adsorbed and/or non-adorbed polymers chains.

GELATION PHENOMENA IN SOFT COLLOIDAL SPHERES

E. STIAKAKIS, D. VLASSOPOULOS, G. FYTAS, A. RISSANOU, I. A. BITSANIS

FO.R.T.H., Institute of Electronic Structure and Laser, Box 1527,
71110 Heraklion, Crete, Greece

Using multiarm star polymers as model colloidal spheres exhibiting ultrasoft interactions, we investigate the interplay of structure and dynamics in the high volume fraction region. We put particular emphasis on the effect of temperature in increasing effectively the star size due to partial swelling in a solvent of intermediate (θ-to-good) quality; this has a dramatic impact in inducing a reversible gelation in such star suspensions. The phenomenon is general as it is observed in a variety of soft sphere – like systems, including dense combs and block copolymer micelles. Using rheological and scattering techniques we identify the role of the molecular parameters in this novel effect, explore its mechanism and propose an alternative ‘jamming’ phase diagram bringing analogies to steric colloids as well as to other states of ‘soft and fragile matter’. Monte Carlo and Molecular Dynamics simulations also suggest a transition to solid-like structures upon temperature-induced swelling and reproduce the increase of G'_{∞}, as well as the freezing of star diffusion. Finally, we study the consequences of nonlinear shearing of the formed gels on the appearance of thixotropic behavior, and examine the gelation in mixtures of soft spheres of soft spheres and linear polymers, in an effort to control this unusual rheological phenomenon.

MODELLING THE INFLUENCE OF MIX PROPORTIONS ON CORRELATION BETWEEN DESTRUCTION PACE AND THIXOTROPY OF SUSPENSIONS

T. LYASHENKO*, V. VOZNESENSKY*, Y. IVANOV**

Odessa State Building and Architecture Academy*
Bulgarian Academy of Sciences**

Investigations of correlation between thixotropic properties of technological mixes and those of mix rheological parameters that could be easily measured would be useful from both theoretical and practical viewpoints. To evaluate the influence of mix proportions on the correlation numerical characteristics would be even more valuable. Though practically unachievable directly from experimental results this has proved to be possible as the result of computational experiment on the fields $Y(\mathbf{x})$ of properties (characteristics Y) of non-Newtonian liquids in co-ordinates of composition factors (vector $\mathbf{x}$), the fields described by experimental-statistical (ES) models and Monte Carlo method used. In this way the influence of composition of building-purpose highly filled disperse systems on flaw behaviour parameters and on correlation between them have been evaluated and analysed. Specifically, when studying silicate system with certain constant cement-sand-water ratio the modification conditions were varied: dosage and type of polyvinylacetate additive (x_1, x_2), dosage and molecular mass of methylcellulose (x_3, x_4), and polypropylene fibre amount (x_5). Physical experiment, using rotational viscometer in range of shear rate from 1 to 134 s^{-1}, was optimally designed, allowing quadratic ES-models for several rheological parameters in dependence of mix proportions to be built. Built on these experimental data, in particular, were structured ES-models presenting the fields of destruction pace of mix structure (m, degree index in Ostwald-de-Waele viscosity model) and relative index of thixotropy (Ω_A) in space of a group of composition factors (for instance, quantity and quality of methylcellulose – x_3, x_4) changing under the influence of factors from another group (dosages of polyvinylacetate and fibre – x_1, x_5). Neither linear nor non-linear significant correlation between m and Ω_A were detected when analyzing the whole bulk of physical experiment data. However, the separation of experimental results into some subsets indicated to possible correlation, changing with modification conditions. To reveal and evaluate the correlation between thixotropy index and destruction pace varying under effects of mix proportions the following computational experiment was carried out.The fields of m and Ω_A in space of composition factors have been simulated. To transform the model-determinate property field into random one the random error, incorporating characteristics of precision of the measurements and ES-model, have been added to Y-level, estimated by corresponding model at each random point (composition) generated. On so obtained sample of pairs $\{m, \Omega_A\}$ estimates of correlation measures (correlation coefficient $r\{m, \Omega_A\}$, regression equation slope, etc.) have been calculated. Multiple generations of the random fields has allowed the distributions for correlation indices to be obtained. At various levels of polyvinylacetate dosage and of fibre amount, in particular, obtained have been the distributions and interval estimates for measures of correlation between the pace of destruction and thixotropy index, revealed through variations of methylcellulose factors. On these results the secondary ES-models have been built describing the influence of composition on degree of correlation. They have allowed the conditions to be defined wherein linear relationship between two criteria is positive, not found, or negative.

ELECTROKINETICALLY ENHANCED FLOW OF COAL-WATER SUSPENSIONS IN PIPES

P.K. ROZAKEAS[1], R.J. SNOW[2]

Faculty of Engineering[2]
Chemical and Metallurgical Engineering Department[1]
RMIT University
GPO Box 2476V
Melbourne, Victoria 3001
Australia.

The transportability and dewatering of coal-water mixtures flowing in a pipe may be enhanced by the application of electrokinetic techniques. Previous experimental work by other workers shows a significant reduction in the wall shear stress, and consequently a decrease in pumping energy requirements for the flow of coal-water mixtures in pipes combined with electrodewatering. In this process the pipe acts the cathode and a centrally aligned tube as the anode. The effects of "in-pipe electrodewatering" on the flow properties and stability of concentrated coal-water mixtures flowing in various alternative anode-cathode arrangements are presented in this paper. The application of an electrical energy flux at the electrode surface (< 6.1 kWm-2) in a dewatering section of pipe (Le = 1m) effectively reduces the pumping energy requirements by as much as an order of magnitude. The stability of flow conditions is investigated in a concentric anode-cathode pipe arrangement consisting of a dewatering and a non-dewatering section (Lo). In this system (Lo/Le) < 4.0. The prediction of flow behaviour in a concentric annulus is also presented. The coal fines (d50 = 17.7 mm used in all experiments were produced by milling a low rank bituminous black coal which was followed by a sieving process that eliminated coal particles that were greater than 75 mm in size.

RHEOLOGY OF DENSE LIGNITE-WATER SUSPENSIONS; PRESHEARING AND TRANSITION STRESSES

THOMAS B. GOUDOULAS, ELEFTHERIOS G. KASTRINAKIS, STAVROS G. NYCHAS

Department of Chemical Engineering, Aristotle University of Thessaloniki
Univ. Box 453, GR-54006 Thessaloniki, Greece
Tel.: +3031996239, +303199623, Fax: +3031996231, +3031996261

An investigation of the rheological properties of dense lignite-water suspensions (LWS) is reported here. The achieved solid volume fraction, ϕ, with acceptable rheological behaviour was 0.45, while the ratio of ϕ/ϕ_m was close to 0.85, where ϕ_m is the maximum solid volume fraction. Systematic viscosity measurements revealed a different behavior of the samples during the ascending and the descending part of applied stresses, in the equilibrium flow curve. The suspension shows a typical thixotropic loop during the implementation of the first flow run, while in consecutive runs the extent of the loop is reduced and a transition point appears with a local maximum. The position of the transition point on the flow curve depends, on the lignite concentration in the slurry and on the number of the consecutive flow runs. The transition stress, σ_{tr}, increases with the number of the runs or the testing time. The value of σ_{tr} increases with total time of testing tending towards a limiting value. It was also observed that σ_{tr} increases with the width of shear stress range. Flow tests were also performed on the LWS with various preshear times and stress levels. The low shear behaviour was found to be quite different from the high shear behaviour for the most concentrated suspensions, with a plateau value at low shear rates indicating a yield stress. These plateau values, however, depend on shear history, which is responsible for the development of different structures in the sample. The non-Newtonian time dependent behaviour of the lignite-water suspensions is attributed to the high value of the ratio ϕ/ϕ_m, the polydispersity of the particle size distribution and the non-spherical shape of the lignite particles.

MODELING SHEAR-INDUCED PARTICLE MIGRATION

LISA MONDY[1], REKHA RAO[1], ROBERT LAGASSE[1], MATT HOPKINS[1], STEVE ALTOBELLI[2], MARC INGBER[3], ANDREA MAMMOLI[3], DAVID FANG[3]

[1]Sandia National Laboratories, Albuquerque, NM 87185-0834
[2]New Mexico Resonance, 2301Yale SE, Suite C1, Albuquerque, NM 87106
[3]Department of Mechanical Engineering, University of New Mexico, Albuquerque, NM 87131

We will give an overview of the performance of a continuum constitutive model of suspensions for low Reynolds number flows. The diffusive flux model (Leighton and Acrivos, *J. Fluid Mech., 1987,* and Phillips et al., *Phys. Fluids A*, 1992) is implemented in a general purpose finite element computational program. The momentum transport, continuity, and diffusive flux equations are solved simultaneously. The formulation is fully three-dimensional and can be run on a parallel computer platform. Recent work introducing a flow-aligned tensor correction to this model has had success in representing the anisotropic force that is seen in curvilinear flows. Gravity effects are added in an approach similar to that of Zhang and Acrivos (*Int. J. Multiphase Flow*, 1994). The model is further refined to allow a time-dependent viscosity to model the polymerization of the suspending fluid.

The model results are compared with laboratory data obtained with Nuclear Magnetic Resonance (NMR) and x-ray imaging of evolving particle concentration profiles in complex flows. NMR results will be shown for noncolloidal, neutrally buoyant particles in various shear flows. Also, batch sedimentation of particles is studied with both imaging methods. The x-ray images are produced after the polymerizing system cures, while the NMR images are obtained in near real time. Both experimental techniques give us particle volume fraction as a function of position, which is then used to validate our numerical results. Results will be shown for three different flow fields: 1) sedimentation in a cylinder with a contraction, 2) sedimentation around a horizontal rod, and 3) sedimentation around a complex three-dimensional shape.

During the computation the viscosity of the polymerizing system can increase by three orders of magnitude. In addition, the systems modeled are highly concentrated (a volume fraction of about 0.48), which leads to stiff equations and numerical instabilities. Interesting secondary flows appear both in the experiment and model. Overall, good agreement is found between the experiments and the simulations. Results have proved useful for a manufacturing application by showing areas likely to trap particles and lead to inhomogeneous material properties.

THE EFFECTS OF PRESSURE AND TEMPERATURE ON THE WALL SLIP PHENOMENON OF DRILLING MUDS

[1]KAYVAN SADEGHY, [2]S. SALIMI, [2]M. KHAIRANDISH

[1]Faculty of Engineering, Department of Mechanical Engineering, University of Tehran, Tehran, IRAN,
P.O. Box: 11365-4563
[2]Research Institute of Petroleum Industry, Tehran, Iran

The effects of pressure and temperature (at levels paralleling those encountered in practice during drilling deep oil and gas wells) on the wall slip phenomenon of Bentonite drilling muds is investigated in this work. A Fann 50C commercial concentric-cylinder viscometer is used to infer information about the slip behaviour of these complex fluids. Using three bobs of the same height but with different diameters, steady shear data were obtained for several straight Bentonite muds at different solid concentrations. A comparison of the flow curves obtained from using different bobs reveals that wall slip was occurring for all test fluids. Steady shear data were also obtained for all test fluids using a Shirley-Ferranti cone-and-plate viscometer. The data from the two viscometers were realized not to be consistent. Because the stress field in a cone-and-plate viscometer is homogenous, it is concluded that slip phenomenon with drilling muds may be of the type of stress-induced-the flow field in a concentric cylinder is not homogenous. To further verify this general conclusion, the slip behaviour of the test fluids was also investigated using a home-built gas-driven capillary viscometer, that is, in a flow where the stress field is definitely inhomogenous. By measuring the driving pressure and the amount of the efflux using two capillaries of the sizes of 1.0 and 1.5 mm, it is demonstrated that slip with drilling fluids is a real issue. These data further supports the idea that drilling muds are vulnerable to wall slip in inhomogenous stress fields. To investigate the slip behaviour of the test fluids under extreme conditions of pressure and temperature, the Fann 50C viscometer was used to obtain steady shear data. By changing the pressure from atmospheric pressure up to 500 psi, and by changing the temperature from room temperature up to 500 deg F, it is concluded that an increase in pressure, reduces the wall slip effects of the test fluids; in contrast, an increase in temperature, is found to have an intensifyineffects of the test fluids. The relation between the slip velocity and the wall shear stress is found to be virtually linear for all test fluids. Tests are currently being carried out to investigate the effect of three polymeric additives (CMC, PHPA and XC), on the slip behaviour of the base Bentonite muds.

TWO-DIMENSIONAL FEM CREEP ANALYSIS OF ORTHODONTIC TOOTH MOVEMENT

CHRISTOPHER G. PROVATIDIS

Mechanical Engineering Department, National Technical University of Athens
9 Heroon Polytechniou Str., GR-157 73 Zografos Campus, Athens, Greece

The biomechanics of tooth movement is still an enigma for both dentists (orthodontists, periodologists, etc.) and computer simulation scientists. Basically, teeth are embedded into the socket (alveolar crest) through the periodontal ligament that operates like a foundation, hydrodynamic [1], elastic [2] or not, of a nearly rigid body. Forces and moments are usually applied on the teeth either during chewing or during orthodontic treatment of adolescents or adults. A reliable mechanical model of tooth movement does not still exist. From the practical point of view, such a model, capable of establishing a reliable relationship between the applied force-system and the induced tooth-movement, would be very useful for many special jobs including those of orthodontists and mechanical engineers. In the future, mechanical engineers could develop specialized S/W to assist decision-making of orthodontists in the optimum forces and moments that should be applied on the teeth through proper orthodontic wires [3]. Linearly-elastic [4-5], viscoelastic [6] and hydrodynamic [7] models of the periodontal ligament have been developed since 1970s by engineers and computer scientists and have been recently critisized by the author. Clinical experiments reveal that the periodontal ligament possesses creep properties but mechanical properties have not been established yet. The aim of this paper is to determine the creep properties of the periodontal ligament using a 2D FEM model of an upper central incisor that has been experimentally studied by Burstone et al. [8]. This was done by firstly digitizing displacement-time curves and further processing that has revealed that these curves are ideally exponential. It was selected that material is modelled using two Young's moduli (E1=linear=0.68MPa, E2=time-dependent) and a viscosity μ. The tooth was considered according to the clinical experiment [8], that is 30 degrees inclined to the vertical plane and a horizontal force of 3N was applied upon it. By trial-and-error the creep properties (E2,μ) were successfully determined.

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VISCOMETRICAL BEHAVIOUR OF SYSTEMS WITH DERMATHOLOGIC AND COSMETIC APPLICATIONS

MARC BARRACÓ-SERRA

Universitat Politècnica de Catalunya

One of the main objectives of the formulation of an emulsion with dermathologic and cosmetic applications is their effectiveness that is characterized fundamentally by their stability.

Several performance strategies exist in this respect, the decreasing of the interfacial stress (by using surfactants) and for increasing their parameters of viscosity (additives).

At the moment they exist a series of additives that, besides their viscosizing character, they present characteristics of biodegradability (the "crimigels").

We present the viscosimetrical behaviour of the following additives:

- Gilucel (Al/Mg hydroxistearat) of lipophilic type
- Stabylen (reticled acrylic copolymer) of hydrophilic nature
- Amigel (glucose homopolysaccharide) of hydrophilic type also.

The present study determines the conditions of good effectiveness for the elaboration and use of these emulsions from the point of view of the classical and preocessing rheoviscometry and from the sensorial aspect.

The determination of the rheoviscometrical characteristics has been carried out in a cone-plate viscometer equipment, Haake VT 550, with control temperature incorporated and data and results computerized.

The sensorial study has been done by a survey carried out a population of hypothetical users, requesting the sensations detected under different application conditions. The general behavior of he has been obtained for statistical treatment of the answers.

The reological and psychorheological parameters provide approaches for an appropriate formulation and effective use.

NONLINEAR DYNAMICS OF DILUTE POLYMER SOLUTIONS

CORNELIA MARIETA CHIUJDEA

University Politehnica Bucharest
77206 Bucharest, Romania

The introduction of small amount of dilute polymers in a turbulent flow changes some mean characteristics of the flow, such as the wall drag that decrease substantially.

Drag reduction by polymer additives is known as Toms effect. The phenomenon of drag reduction was discovered by B.A.Toms in 1946 by chance when he investigated the mechanical degradatioin of polymers using a pipe flow apparatus and noticed that the polymer solution offered less resistance to flow in turbulent conditions under constant pressure that the solvent itself.

At present dilute polymer solutions are well known to be non-Newtonian fluids and from anlysis of rheological properties results that they are shear thinning materials which manifest a substantial elongational viscosity. A polymer solution even a very dilute one can be regarded as a viscoelastic fluid.

In viscoelastic flows the wall turbulence regeneration is influenced by the mean shear and by the interaction of the coherent structures even if they appear more ordered and larger with respect to Newtonian flows. The analysis of data from analytic and numerical solutions of the flow equations together with a rheological model for the polymer solutions suggest as the main effect of the viscoelastic charateristics is a stabilizing action on the low speed streaks and the decreasing level activity of the wall layer coherent structures. These mean important changes in the scale of turbulence and originate the drag reduction phenomenon.

In this paper the effect of rheological properties of dilute polymer solutions on the near wall turbulent flow is studied on the basis of a three- dimensional nonlinear sinusoidal model of turbulent motion. The processes leading to such behavior are very complex and studing the turbulence of such complex flow fields are very complicated.

The results of this investigation of drag reduction phenomenon on dilute polymer solutions make it possible for us to formulate a possible physical mechanism of the effect of polymer molecules on the turbulent flow.

Our main conclusion is that despite of the great number of theories that have been proposed to explain the drag reduction effect, the existing theories are inadequate of explaining the phenomenon exhibits itself in the experiments. We believe that the research in this area has to continue.

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A TEMPORAL NONLINEAR STABILITY ANALYSIS OF VISCOELASTIC CHANNEL FLOWS

KUNT ATALIK, ROLAND KEUNINGS

CESAME, Division of Applied Mechanics, Université catholique de Louvain
B-1348 Louvain-la-Neuve, Belgium

The stability analysis of infinitesimal and finite disturbances to fluid flows using linear and nonlinear approaches respectively, and the details of the transition mechanism from laminar to turbulent regime are still an active research topic even for classical Newtonian fluid flows. It has been known that viscoelastic contributions alter and enrich this transition picture in the limit of high Reynolds number. Recent experimental investigations with viscoelastic fluids indicate another loss of stability due to purely elastic effects in the limit of inertialess flow and the possibility of elastic turbulence. In recent years, several linear stability analyses in the case of plane channel Poiseuille and Couette flows did not show any loss of stability although the numerical treatment of the equations caused severe problems with the detection of artificial instabilities.

In this study, it is aimed to conduct a nonlinear analysis of finite two- and three- dimensional disturbances in channel Poiseuille and Couette flows for viscoelastic fluids using the upper convected Maxwell and Oldroyd-B models. Shear thinning effects are considered by the inclusion of a Giesekus term in the equations.

In the two-dimensional case, the streamfunction formulation is used whereas in the three-dimensional case the primitive variable formulation with the choice of a divergenceless velocity field, which effectively eliminates the pressure variable, is preferred. The Fourier-Chebyshev spectral decomposition of the flow variables is used and the Galerkin spectral method is applied to obtain a finite-dimensional dynamical system governing the time evolution of the disturbances. A Crank-Nicholson Adams-Bashforth mixed scheme is used for the time integration of the dynamical system. Initial conditions are formed from the most unstable eigenmodes of the corresponding linear stability problem.

The transition mechanism is discussed in terms of both the transient linear growth of the misfit disturbances due to the nonnormality of eigenmodes and the nonlinearity effects.

The effects of elasticity on high Reynolds number flows, i.e. the destabilization of disturbances followed by a stabilization with increasing elasticity, are first discussed with reference to drag reduction phenomena. Then in the low Reynolds number limit, the search for the possibility of the bifurcations in two and three space dimensions with the increase in Weissenberg or Deborah numbers, leading from the laminar state to finite-amplitude periodic structures and to elastic turbulence, is addressed in terms of the temporal nonlinear evolution of the disturbances.

NUMERICAL SIMULATIONS OF GENERALIZED NEWTONIAN FLOWS INVOLVING TWO FREE SURFACES

GEORGIOS GEORGIOU*, PHILIPPE LEMENN, ANDREAS ALEXANDROU****

*Department of Mathematics and Statistics, University of Cyprus, P.O. Box 20537, 1678 Nicosia, Cyprus
**Mechanical Engineering Department, Worcester Polytechnic Institute, Worcester MA 01609-2280, USA

Generalized Newtonian flows involving two free surfaces are analyzed by means of the finite element method and the full-Newton iteration scheme. We will first present results for the steady, annular Newtonian liquid jet flow at high Reynolds numbers obtained for various values of the inner to the outer diameter ratio using extremely long meshes. The annular film moves far from the symmetry axis at low values of the Reynolds number. At higher Reynolds numbers, the film moves towards the axis of symmetry and appears to close very far downstream, forming a round jet. Asymptotic results for the radius of the resulting round jet will also be provided.

The second flow we consider is the time-dependent flow of non-symmetric Herschel-Bulkley films impinging on a wall, which is related to the filling of a two-dimensional cavity. The effect of various parameters, such as the yield stress, the Reynolds number and the power-law index, on the stability of the flow will be investigated.

STRESS-INDUCED MIGRATION EFFECTS ON THE TAYLOR-COUETE FLOW OF A DILUTE POLYMER SOLUTION

M.V. APOSTOLAKIS,[1] V.G. MAVRANTZAS,[1], A.N. BERIS[1,2]

[1]Institute of Chemical Engineering and High-Temperature Chemical Processes (ICE/HT-FORTH)
Patras, GR 26500, Greece
[2]Department of Chemical Engineering, University of Delaware, Newark, DE 19716, USA

Stress-induced polymer diffusion was first observed and reported by Shafer et al.[11] and Dill and Zimm[4] who published convincing evidence about the radial migration of high MW DNA molecules in solutions subject to flow between concentric cylinders or cones for long times (on the order of many hours to a day). In the subsequent years, the phenomenon was modeled using either kinetic theory arguments based on the elastic dumbbell model or continuum models based on various formalisms (body tensor, anisotropic kinetic theory, two-fluid Hamiltonian and projection methods).[1-3,5-10] The significance of the effect in usual viscometric flows was analyzed by Mavrantzas et al.[7] who solved the entire set of governing equations (diffusion, momentum and constitutive) in a generalized viscometric device consisting of a stationary lower plate separated a non-zero distance by a rotating upper cone. In the present work, the stress-concentration coupling effects are analyzed in the Taylor-Couette device, consisting of two infinitely-long concentric cylinders. The underlying molecular model is a two-fluid Hamiltonian model, consisting of two components, one of which is viscoelastic and obeys the Oldroyd-B constitutive equation. The two components of the mixture are considered to be in thermal but not mechanical equilibrium interacting with each other through a drag coefficient tensor. The solution to the steady-state purely azimuthal flow is first addressed with a spectral collocation method and an adaptive mesh formulation to track the steep changes of the concentration in the flow domain. The numerical results show substantial migration of polymer from the outer to the inner cylinder in agreement with the experimental data. The migration is enhanced for decreasing gap thickness values and increasing Deborah numbers. It also depends on the solvent to polymer viscosity ratio. When the contribution of the polymer viscosity is significant, the effect of the stress-induced concentration gradients on the flow kinematics is important. At high Deborah numbers, the dramatic depletion created in the area near the outer cylinder is accompanied by significant deviations in the velocity profile from its form corresponding to a uniform concentration. Results will also be reported from a linear stability analysis of the inhomogeneous steady-state profiles corresponding to various wavenumbers in θ and z direction.

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NUMERICAL SIMULATION OF THE PLANAR CONTRACTION FLOW OF THE OLDROYD-B FLUID

L. SAOUDI(*), N. ZERAIBI(**)

*Institut de Physique, Laboratoire de Mécanique des fluides, USTHB.
**Faculté des hydrocarbures et de la chimie Université de Boumerdes
Fax (02) 24-73-44

The flow of the Oldroyd-B fluid through an abrupt contraction is analyzed by means of finite difference. In discretizing the continuity, momentum and constitutive equations on a uniform grid system. different schemes are used like Upwind difference scheme and Central difference scheme.

In the present study, after resolution of the whole system of the governing equations and the boundary conditions by numerical simulation, we present the results of this work by analyses the distributions of a stream function, a vorticity and a first normal stress; we then discuss the effects of inertia and elasticity upon the corner vortex size and the location of the center of rotation.

Keywords: Effect of inertia; effect of elasticity; Oldroyd-B fluid; planar contraction flow; UD scheme; CD scheme; Reynolds number; Weissenberg number.

MODELING OF VISCOPLASTIC LID-DRIVEN CAVITY FLOW USING FINITE ELEMENT SIMULATIONS

E. MITSOULIS, M. BEAULNE, D. KAMMER, A. ZISSIS

Dept. of Mining Eng. & Metallurgy, National Technical University of Athens, GREECE

Numerical simulations are undertaken for the benchmark problem of lid-driven cavity flow, with the objective to give accurate solutions for viscoplastic fluids. The rheological constitutive equation employed is a continuous viscoplastic model, which can be made to mimic the ideal Bingham plastic model as closely as desired [1]. The simulations are undertaken for the whole range of Bingham numbers (Bn) from 0 (Newtonian fluid) to infinity (undeformed plastic) and various cavity aspect ratios, employed previously in similar simulations but for viscoelastic flows [2].

The numerical results show the extent of the yielded/unyielded regions in the cavity as the Bn increases. The lower part of the cavity becomes unyielded and also the part around the eye of the vortex. However, there always exist yielded regions in the upper part close to the lid, due to the lid motion. The unyielded island close to the lid becomes larger with increasing Bn and moves closer to the lid. The eye of the vortex also moves closer to the lid. The numerical solutions give the location and intensity of the vortex as a function of Bn number. These results serve as benchmark solutions in this prototype flow.

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PARTICLE SINTERING AND MELT DENSIFICATION IN ROTATIONAL MOLDING

J. VLACHOPOULOS*,C. BELLEHUMEUR, M. KONTOPOULOU*****

* Chemical Engineering,McMaster University
University of Calgary,*Queen's University
CANADA

The rotational molding process involves the tumbling and heating of polymer powders in a rotating mold. Under such conditions the polymer particles tend to decrease their surface area by coalescence (sintering).The initial stage of this process was described mathematically on the basis of Frenkel's model involving the surface tension which is counteracted by viscosity. This model was subsequently modified to better describe the experimental observations over a wider range and to include viscoelasticity. The bubbles that get entrapped in this process, eventually diffuse and disappear in the melt. The experimental results were compared to predictions of some models used in ceramic and metal densification processes and were found to be in relatively good agreement. A bubble dissolution model was developed for the description of the late stages of the densification .The combination of models is capable of predicting the whole process from the moment when molten particles first contact each other to the point where the melt reaches the density of solid for some polymers. Experimentally some differences were noted in the densification phenomena due to different levels of crystallinity and elasticity.

VISCO-ELASTIC MODELLING OF MICRO-INJECTION MOULDING

C. JEGGY, F. DUPRET

CESAME, Université catholique de Louvain, Louvain-la-Neuve, Belgium

Micro-injection moulding is a relatively new polymer processing technology. It derives from classical injection moulding, but, in this particular case, the mould comprises micro-cavities whose size is of the order of the micron and exhibits a fully three-dimensional aspect. As a consequence, the filling of these micro-cavities and the demoulding of the part represent major process difficulties and filling prediction via numerical simulation is therefore crucial.

Because of the fully three-dimensional aspect of the micro-cavities, the Hele-Shaw approximation (which consists in neglecting one part dimension in front of the other two dimensions) is no longer valid in micro-injection modelling.

On the other hand, observations of experimental results clearly indicate that flow instabilities often occur during filling. An investigation of the importance of viscoelastic effects has been conducted and shows that visco-elasticity can not be neglected in micro-injection moulding. We have thus turned our attention to visco-elastic models for the prediction of the polymeric flow. The Giesekus model, which gives a nonlinear constitutive equation for the extra-stress tensor, has been chosen after some investigations.

The numerical method that we have adopted for solving this unsteady visco-elastic problem is related to the alternating implicit technique of P. Saramito ("A new scheme algorithm and incompressible FEM for viscoelastic fluid flows", Math. Modelling Num. Anal. , 28 n°1, 1994, p. 1 à 34), where the time step is divided into 3 substeps with a θ parameter. This method requires to solve at each time step two Stokes-type subproblems and one transport-type subproblem and thus results in decoupling elastic and viscous numerical integrations.

RHEOLOGY OF POLYTETRAFLUOROETHYLENE IN PASTE EXTRUSION

ALFONSIUS B. ARIAWAN, SAVVAS G. HATZIKIRIAKOS

Department of Chemical Engineering, The University of British Columbia
2216 Main Mall, Vancouver, BC, V6T 1Z4, CANADA

The rheology of polytetrafluoroethylene (PTFE) pastes has been studied using a simple Instron capillary rheometer equipped with two barrels of different sizes. Four different grades of PTFE have been tested. Three of them had a homopolymer structure with different molecular weights. The fourth polymer had a slight degree of branching due to the incorporation of about 0.1% by weight of another perfluorinated monomer. The investigated parameters included those related to the die design (cone contraction angle, capillary diameter and capillary length to diameter ratio), extrusion conditions (temperature, lubricant content, and extrusion speed) and the molecular weight and structure of PTFE. It was found that all these parameters significantly affected the extrusion pressure, which is a strong indication of the extent of fibrillation that has occurred during the paste extrusion. Higher pressures generally resulted in the formation of stronger extrudates. Too high of a pressure, however, tended to break the fibrils and rendered the extrudate weaker. Quantification of the amount of fibrillation in the extrudate has been attempted by the use of Raman microscopy. An attempt has also been made to correlate the degree of fibrillation with the tensile strength of the extrudate.

Key words: paste extrusion, teflon, fibrilation, capillary rheometry

THE INFLUENCE OF COMPLEX RHEOLOGICAL PROPERTIES ON MIXING

LIDIJA SLEMENIK, ANDREJA ZUPANČIČ, MIHA ŽUMER

University of Ljubljana, Faculty of Chemistry and Chemical Technology, Department of Chemical Technology,
Chair of Chemical, Biochemical and Ecological Engineering,Aškerčeva 5, SI-1000 Ljubljana, Slovenia
phone: +386 1 476 04 23, fax: +386 1 426 45 77

Mixing of rheologically complex fluids occurs in a wide variety of industrial processes. Mixing process can be very complicated when the medium exhibits complex rheological properties like viscoelasticity, the yield stress and irreversible time dependence of viscosity during shear action. Turbulence can hardly be achieved during mixing highly viscous fluids so the operation is often performed in laminar flow regime.

The present work deals with mixing of highly viscous fluids with non-newtonian rheological properties. The mixing process of complex fluids was investigated in a flat-bottomed cylindrical plexiglass vessel. The vessel had a 0.19 m diameter and no baffles. The ratio between the height of the liquid and the diameter of the vessel was equal to 1. Mixing was performed with several impellers in laminar flow regime. Special emphasis was laid on mixing with helical ribbon impeller. Due to very large diameter, which was very close to the inside diameter of the vessel, the helical ribbon impeller guaranteed liquid motion throughout the vessel. Mixing efficiency was evaluated with measurements of power requirement and mixing time. Mixing time was determined with thermal response technique and flow visualization method. Photographs were taken to follow the generation of flow patterns. To evaluate the effect of rheological complexities on mixing process different Newtonian and non-Newtonian fluids were used. Aqueous solutions of the fluids were prepared in different concentrations at ambient temperature. The rheological properties of the fluids were examined with two rotational rheometers at different temperatures. The same rheological tests were investigated before, during and after mixing process.

Keywords: mixing, mixing time, power requirement, helical ribbon impeller, rheology, high viscosity fluids

DYNAMICAL PROCESS OF POLYELECTROLYTE GEL SWELLING - SWELLING CONTROLLED SOLUTE RELEASE

EVDOKIA C. ACHILLEOS, KOSTAS N. CHRISTODOULOU,
IOANNIS G. KEVREKIDIS

A multi-dimensional, multi-component model for the swelling of polyelectrolyte gels in salt solutions, which accounts for the effect of network stress, osmotic pressure, and electrical potential on the species diffusive flux, and accounts for the mixing, elastic, and electrostatic free energy (1,2) is applied here to study applications of solvent transport of polyelectrolyte gels which have a strong transient character. The mechanical response of gel swelling and de-swelling under application of external solution composition fluctuations was simulated. The predicted average gel height at the periodic steady state was found to be different from the one corresponding to the average forcing (composition). The other dynamical process studied was swelling-controlled solute release. Simulations of solute release from finite volume gel cylinders of different aspect ratios with simultaneous gel swelling were performed. These simulations predicted that the time dependent solute release is a strong function of the gel geometry, swelling rate, and degree of swelling.

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MULTI-SCALE THERMOPLASTIC FOAM RHEOLOGY MODELING

JAAP DEN DOELDER

Dow Benelux N.V.
P.O. Box 48
4530 AA Terneuzen
The Netherlands

The first part of the talk will be a general overview of the R&D activities of The Dow Chemical Company. Emphasis will be put on developments involving the field of rheology. The second and main part of the talk will be an in-depth presentation of the author's recent work on modeling foam growth in thermoplastic materials. A model is presented that consists of two elements. The first element follows the growth of single bubbles, beginning when they are microscopically small in a post-nucleation state, up to the point where growth stops. This involves bridging length scales from submicrons to millimeters. The parallel second model element calculates continuum heat and concentration diffusion through a growing foam board, reaching a length scale of centimeters. The actual bubble size distribution at a given time influences the material parameters of the continuum level model, whereas simultaneously the macroscopic temperature and concentration distribution acts on the local bubble growth dynamics. The models serve to speed-up new product development by reducing the need for experiments. Typical results for a PolyStyrene foam are presented.

MORNOS: A LEADING GREEK PLASTICS PACKAGING COMPANY

D. GIANNAKIDIS

MORNOS S.A
7th km Thiva-Chalkida, P.O.B. 134, GR-322 00 Thiva, Greece

MORNOS, one of the leading Greek plastics packaging converters, which belongs to the K. Filippou Group, is looking positively into the future.
A perspective of the type of management applied at MORNOS and the handling of various technical problems will be viewed:

- How the MORNOS team operates.
- Handling new product developments, communicating with suppliers, solving customer technical problems, solving internal technical problems.

SOLITARY WAVE DYNAMICS OF NEWTONIAN FILM FLOWS: EXPERIMENT AND SIMULATION

M. VLACHOGIANNIS, N. MALAMATARIS, V. BONTOZOGLOU

Department of Mechanical & Industrial Engineering
University of Thessaly, Pedion Areos
GR-38334 Volos, Greece
(Phone: +30421 74069, Fax: +30421 74050)

The spatio-temporal evolution of an inclined or vertical falling film is a classical open-flow problem with significant engineering applications. Nonlinear evolution of the unstable free surface has been the focus of recent experimental and theoretical research. Imposing inlet disturbances of controlled frequency, Liu &Gollub (1994) showed that high-frequencies lead to saturated periodic waves, whereas low-frequencies produce solitary waves. They also documented the interaction between solitary humps resulting in coalescence. Chang et al. (1995) analyzed by dynamic systems techniques a simplified equation based on the long-wave approximation and made further predictions for the dynamics leading to and emanating from coalescence events. In the present work, we report on recent progress in the experimental study of solitary wave interactions and in the simulation of the pertinent dynamics by directly solving the Navier-Stokes equation of motion.

A fluorescence imaging technique is used to capture the spatio-temporal evolution of inclined film flow. By systematically recording numerous coalescence events, we show that the duration of the merging process depends inversely on the difference in height between the interacting humps. Thus, similar waves may resist coalescence and form double-hump pulses. Transient phenomena accompanying coalescence are documented. In particular, the excited hump (resulting from merging) is found to develop an elevated back-substrate, whose height scales with the crest elevation and which decays exponentially in time. The elevated back substrate is stable for viscous liquids, but in experiments with water it readily gives in to a tail modulation. If the wave is isolated, the modulation lags behind the crest and decays. If, however, a second wave follows, the tail modulation may be trapped in-between and nucleate a new hump.

Numerical simulations are also performed, using a Galerkin finite-element method and imposing disturbances of controlled frequency at the computational inlet. The experimentally recorded dependence of the evolution on frequency (from the linear growth rate to the final stationary form) is recovered quantitatively and new predictions are made about the velocity field produced by large solitary waves. Finally, by artificially introducing solitary humps of different size, we are able to simulate wave-wave interactions and put them in perspective with the data.

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TWO-PHASE FLOW IN AN UNDULATING TUBE: TRANSITIONS FROM STRATIFIED TO DISCONTINUOUS FLOW OF ONE OF THE FLUIDS

Ch. KOURIS, J. A. TSAMOPOULOS*

Laboratory of Computational Fluid Mechanics, Department of Chemical Engineering, University of Patras

Our goal is to simulate the different two-phase flow regimes, which arise in the operation of packed bed reactors or, generally, in porous media. For example, the pulsing flow regime is characterized by continuous flow of the fluid that wets the catalytic particles and discontinuous flow of the fluid that occupies the remaining void space. To this end, the dynamics of the two-phase flow in a tube is examined, the radius of which varies sinusoidally in the axial direction and for such values of the operating parameters that linear theory predicts [1], [2] and experiments demonstrate [3] that the stratified flow is unstable. The required simulations must accommodate topology changes of either phase. This can be accomplished by the Volume of Fluid (VOF) method for the calculation of the flow field and the fluid/fluid interface, [4], [5]. The governing equations of both fluids are approximated by central finite differences in a staggered mesh. The effect of surface tension is accounted for according to Brackbill et al. [6]. The explicit Euler method has been used to integrate for long times or until the system reaches a stable limit cycle. Important flow parameters are the volume fraction of the tube occupied by the inner fluid, V, the viscosity, μ, and density, ρ, ratio of the two fluids and the *Re* and *Ca* numbers. Our results demonstrate that decreasing V induces transition from stratified flow to discontinuous flow of the core fluid, which forms slugs dispersed in a continuous stream of the annular fluid. Figures 1 and 2 give the interface between the two fluids and the solid boundary at two different time instants, t=4.2 and 6, and for parameter values leading to slug formation. Smaller drops are formed, when V decreases further. A different transition is that from the stratified flow to the spray regime and occurs as the importance of the surface tension decreases. In that case, small ripples develop on the interface, which grow forming fingers pointing towards the less viscous fluid. Eventually small drops of the more viscous fluid are broken up and get immersed in the other fluid. The importance of the various parameters is studied.

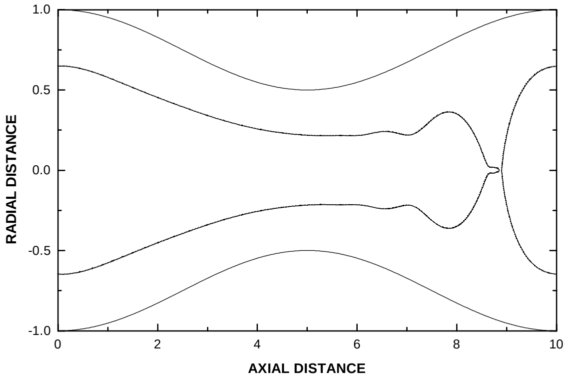

Figure 1

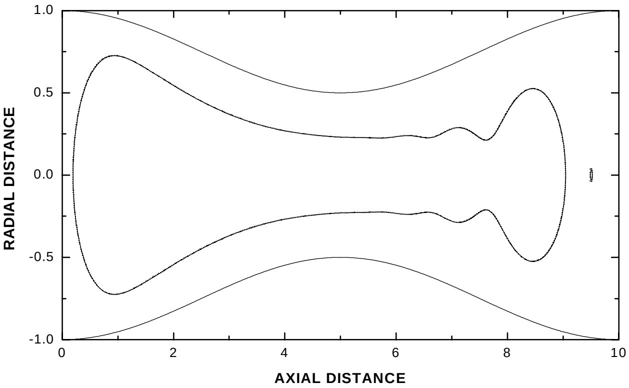

Figure 2

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ANALYZING ACRIVOS' EXPERIMENTS WITH FINITE ELEMENTS

D.P. PAZIS, N.A. MALAMATARIS

Dpt. Mechanical & Industrial Engineering
University of Thessaly
38334 Volos, Greece

The steady flow in rectangular cavities of finite and infinite depth and of Reynolds numbers ranging from the limit of Stokes flow up to 4000 has been the subject of Professor Acrivos' experiments in the 60's (Pan and Acrivos 1966). Despite the progress in computational fluid mechanics in the last decades and the many attempts to develop benchmark solutions for this flow, there are still many issues unaddressed from a computational point of view like how the size of the eddies is affected by a continual increase in the Reynolds number or how Batchelor's (1956) mean square law could be convicingly confirmed.

In this work, we are going to approache these unsettled questions using the Galerkin finite element method in primitive variable formulation. The numerical results are in good agreement with the available experimental measurements obtained by Pan and Acrivos and the numerical analysis of the magnitude of the vorticity in the flow yields reliable data. Additional numerical results are shown for the separated flow over an inclined fence, which are in good agreement with Taneda's (1979) experiments. The analysis shows how shear stress and vorticity change along the fence and the wall for various fence inclinations. For small inclinations the flow around a fence may also be considered as a cavity flow showing similar behavior with the results of Acrivos' experiments.

LOW REYNOLDS NUMBER TURBULENT CHANNEL FLOW

D. JANKOVIC, A.N. BERIS*, R. KEUNINGS, G.S. WINCKELMANS

CESAME, Université catholique de Louvain, Louvain-la-Neuve, Belgium
*Dept. Chem. Engng., Univ. of Delaware, USA

In this work we investigate the turbulence structure in channel flow at low Reynolds numbers through Direct Numerical Simulations (DNS). The solutions are obtained though parametric continuation as the friction Reynolds number is gradually decreased from a value of 125. This technique allows to obtain turbulent flow solutions for much lower friction Reynolds numbers and thus study more closely the long term stability of turbulent structures and their ultimate transition to laminar flow.

Albeit the calculations performed so far are for a Newtonian fluid, the long term objective of our work is to study viscoelastic turbulent flow and in particular, if possible, whether we can obtain viscoelastic inertialess turbulence such as that observed in recent experiments in viscometric flows with dilute polymer solutions.

We plan to use there the same strategy whereby a family of numerical solutions is computed for decreasing values of the Reynolds number, from the inertia-driven turbulent regime down to the elasticity-driven turbulent regime. The issue of initial guess is therefore a critical one, for which we propose here a suitable interpolation method.

In this study we use a semi-implicit, time-splitting spectral method implemented on a 16-node Beowulf pc-cluster parallel computer. The Newtonian simulations reveal that when reached from higher Reynolds numbers, the transition from turbulent to laminar flow occurs at a friction Reynolds number of about 65, which corresponds to a mean flow Reynolds number of 900.

DOUBLE REPTATION PREDICTIONS OF THE LINEAR VISCOELASTICITY OF MELT MISCIBLE POLYMER BLENDS

JAI A. PATHAK, RAMA KANT, SANAT K. KUMAR, RALPH H. COLBY

Materials Science and Engineering
The Pennsylvania State University
University Park, PA 16802 USA

Using a concentration fluctuation model, we first predict the distribution of segmental relaxation times for each component in melt miscible polymer blends from experimental determination of those fluctuations using small angle neutron scattering data. This prediction relies on a temperature dependent phenomenological form for the size of the cooperative volume required for segmental motion. The predicted segmental time distribution is sampled to determine the average longest segmental relaxation time of each chain, which is taken to be the effective Kuhn monomer relaxation time of the tube model. The reptation scaling of de Gennes determines the terminal relaxation time of each chain in the blend from this effective Kuhn monomer time and the number of monomers per chain, using a single reciprocally-averaged tube in the blend. The double reptation model of des Cloizeaux is used to predict the linear viscoelastic stress relaxation modulus of the blend. This time dependent modulus is then transformed to the frequency domain to predict the storage and loss moduli of the blend. While these calculations are not trivial, they predict the linear viscoelastic response of melt miscible polymer blends from knowledge of their concentration fluctuations (measured by neutron scattering) and their pure component dynamics and chain lengths, with no adjustable parameters apart from the assumed temperature dependence of the cooperative size.

This model is first tested using miscible blends of 1,4-polyisoprene and polyvinylethylene. Segmental dynamics in this blend has been studied extensively using 2D solid state NMR by Kornfield, and the experimental distribution of segmental relaxation times of each blend component is compared with the predictions of the concentration fluctuation model. Roovers and Toporowski have measured the storage and loss moduli of several blend compositions at various temperatures. The double reptation predictions qualitatively predict these data. The local maxima in the loss modulus at low frequency are reasonably described in terms of both composition and temperature dependence. In particular, the failure of time-temperature superposition reported by Roovers and Toporowski is predicted well by the model. The utility of the model for other melt miscible polymer blends will also be discussed, along with the reasons why the model lacks quantitative predictive powers at present.

QUANTITATIVE THEORY FOR LINEAR RHEOLOGY OF LINEAR ENTANGLED POLYMERS

ALEXEI E. LIKHTMAN*, TOM C.B. MCLEISH

Polymer IRC, Physics Department, University of Leeds, Leeds LS2 9JT, UK

We present a new quantitative development of the reptation picture of de Gennes-Doi-Edwards. It is well known that the original reptation theory is unable to fit linear relaxation spectra (G' and G'') as it misses several important physical processes: 1) contour length fluctuations, 2) constraint release, 3) longitudinal stress relaxation along the tube. All of these processes were treated theoretically before; however the treatment used either uncontrolled approximations or failed to include all of them at the same time.

The aim of this work is to combine self-consistently theories for contour length fluctuations and constraint release with reptation theory. First we improve the treatment of chain length fluctuations using combined theoretical and stochastic simulation approach. This allows us to obtain an expression for the single chain relaxation function $\mu(t)$ without any adjustable parameters and approximations. To include constraint release we use the scheme proposed by Rubinstein and Colby (1988), which provides an algorithm for calculating the full relaxation function G(t) from the single chain relaxation $\mu(t)$. Then longitudinal modes are added and detailed comparison with different experimental data is given.

A GENERIC FORMULATION OF TWO-PHASE FLOW

MARKUS HÜTTER, HANS-CHRISTIAN ÖTTINGER

Department of Materials, Institute of Polymers, ETH Zürich, CH-8092 Zürich, Switzerland

A two-phase model is developed using the GENERIC (general equation for the nonequilibrium reversible irreversible coupling) formalism [1, 2]. The description we propose has the following properties. First, it allows to use the thermodynamic potentials of the two individual phases. Hence, it is possible to consider the effects of temperature differences, of chemical potential differences, and of pressure differences between the two phases. Second, the interface separating the two phases is characterized in terms of the temperature dependent surface tension. Third, the two phases are assumed to move at the same velocity and hence only one momentum balance equation instead of two is needed. And fourth, the volume fraction and the interface density (amount of interfacial area per volume element) are the key variables in the system. In the current description the set of variables are therefore the mass density, the momentum density, and the internal energy density of the mixture, the mass density and the internal energy density of one of the two phases, the internal interfacial energy density, and the topological parameters volume fraction and interface density. The formulation of the energy and entropy functionals needed in the GENERIC framework is straightforward in the sense that both are the sum of the corresponding contributions of the individual phases plus a contribution due to the surface tension. It is noteworthy that using this entropy functional, the functional derivatives include the temperature differences, of chemical potential differences, and of pressure differences between the two phases in a natural manner. In order to find the reversible contribution to the equations, the Poisson operator L is constructed based on the transformation behavior of the variables under space transformations. The resulting L-operator is antisymmetric (by construction) and fulfills the Jacobi-identity. Furthermore, the functional derivative of the entropy lies in the null space of L as required. Apart from the purely convective terms in the reversible equations, a surface tension contribution appears in the momentum balance which can naturally be incorporated into the stress tensor expression. However, one should note that the expression for this surface tension contribution is different than what is commonly used in the corresponding literature. As far as the irreversible dynamics is concerned, the following contributions to the balance equations have been considered. First, the viscous stress effects are incorporated assuming that both the mixture as well as one of the two phases behave as Newtonian fluids. Second, the heat transport in the bulk of the two phases is implemented according to Fick's law. Third, in addition to the previously mentioned heat transport within each of the phases, a mechanism to achieve thermal equilibration in the whole system is necessary. Since generally the temperatures of the phases differ from each other, the heat exchange between the two phases across the interface is modeled to enable temperature equilibration. The resulting expressions correspond to the equations used in literature. For all three contributions discussed above, the corresponding (metric) M-matrix used in GENERIC is Onsager-Casimir symmetric and positive semi-definite, and fulfills the degeneracy requirement that the functional derivative of the energy lies in the null space of M (energy conservation). It is also shown that a common approximation for this heat exchange through the interface must be handled with care since the corresponding M-matrix is only positive semi-definite if certain conditions are fulfilled.

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NON-NEWTONIAN RHEOLOGY OF ENTANGLED POLYMER SOLUTIONS AND MELTS

CHRISTOS TSENOGLOU

Dept. of Chemical Engineering / Polymer Technology Lab.
National Technological University of Athens.
157-80 Zografou, Greece

Molecular theory based scaling arguments relating the extent of entanglement depletion to the prevailing flow intensity are utilized for the quantitative description of the shear thinning rheology of entangled linear polymer solutions and melts. A power law decay with respect to shear rate ($\dot{\gamma}$) is assumed for the viscosity, $\eta \sim K\dot{\gamma}^{n-1}$, and the first normal stress coefficient, $\Psi_1 \sim L\dot{\gamma}^{m-2}$. Following experience and the Doi-Edwards molecular theory, the lower rate limit of the non-Newtonian regime is taken equal to the inverse of the relaxation time of the whole chain. By analogy, and consistent with Menezes and Graessley's model for polymer relaxation under fast flow, it is assumed that shear thinning ceases at a characteristic higher rate equal to the frequency of the swiftest entanglement renewal process. Within these two $\dot{\gamma}$ limits which define the non-Newtonian regime, estimates for the n and m exponents are made connecting them to molecular relaxation characteristics. Expressions for the K and L coefficients are also derived, relating them to the molecular weight, chain rigidity, polymer concentration and temperature.

CHAIN CONFORMATIONS AND FORCES IN PHYSISORBED LAYERS OF HOMOPOLYMER COLLOID STABILIZERS: COMPARISON BETWEEN MONTE CARLO AND MEAN FIELD PREDICTIONS

JASON DE JOANNIS[1], JORGE JIMENEZ[1], RAJ RAJAGOPALAN[1], JOANNE THOMATOS[2], IOANNIS A. BITSANIS[3]

[1]Department of Chemical Engineering, University of Florida, Gainesville, FL, USA
[2]Interchem Hellas, R & D Department, Vathi Avlidos, Evia, Greece
[3]FO.R.T.H. – I.E.S.L., Vassilika Vouton, Heraklion, Crete, Greece

We present a systematic comparison between results of lattice Monte Carlo (MC) simulations and predictions of the lattice mean field theory (MF) of Scheutjens and Fleer for homopolymers physisorbed on solid surfaces. The Monte Carlo simulations became feasible by the development of an extension of the Configurational Bias method. The comparison included both detailed (i.e., polymer volume fraction profiles) and global features (i.e., layer thickness and adsorbed amount) of the physisorbed layer.

Typical homopolymer stabilizers with M.W. between 10^4 – 10^5 (100 – 1,000 lattice segments) are too short to follow asymptotic power law predictions. The quantitative differences between MC and MF polymer concentration profiles are substantial (locally up to factors of 10) with MF underestimating the polymer concentration. This results in significant differences for the adsorbed amount and layer thickness, which are pronounced for adsorption from dilute solution. The MC results for longer chains are consistent with scaling power laws and illustrate the self-similar structure of the intermediate part of the adsorbed layer.

The development of a new methodology (Contact Distribution Method) made possible the first calculation of forces between surfaces in lattice MC simulations, under conditions of restricted equilibrium. The simulation findings show the importance of excluded volume forces, even for single chain adsorption. The shift from attractive to repulsive forces takes place at a relatively low degree of surface saturation. MF calculations underestimate systematically the repulsive contribution to the surface forces. Scaling of the distance with the unperturbed layer thickness leads to collapse of the force – distance profiles with the same degree of relative surface saturation.

PREDICTION OF THE RHEOLOGICAL PROPERTIES OF LONG POLYETHYLENE MELTS VIA ATOMISTIC SIMULATIONS

V.A. HARMANDARIS,[1,2] V.G. MAVRANTZAS,[1] D.N. THEODOROU[1,2]

[1]Institute of Chemical Engineering and High-Temperature Chemical Processes (ICE/HT-FORTH), and
[2]Department of Chemical Engineering, University of Patras, GR 26500, Greece

A systematic effort has been undertaken to predict the viscoelastic properties of polyethylene (PE) melts through a hierarchical approach which entails detailed atomistic Monte Carlo (MC) simulations of oriented systems followed by molecular dynamics (MD) simulations. The approach consists of three stages:

Stage I: Here, the representation of the melt is coarse-grained by defining a global descriptor of its overall configuration, the conformation tensor **c;** this is assumed to develop in response to an externally imposed tensorial field **α**. In the present work, the field **α** has been taken to correspond to a steady-state uniaxial elongational flow along the *x* axis. For a given value of **α**, a detailed atomistic end-bridging Monte Carlo (EBMC) simulation is performed [Mavrantzas and Theodorou 1998; 1999; 2000]. This allows us to sample a sufficient number of fully equilibrated, oriented melt configurations characteristic of the system structure under the applied flow field.

Stage II: The dynamics of the melt systems is studied in this stage by performing long MD simulations starting from the atomistic configurations sampled in Stage I. Two different approaches are followed:

- The first involves MD of *equilibrium configurations*, sampled during EBMC simulations at a zero field, in the NVT statistical ensemble [Harmandaris *et al.,* 1998]. To reduce the problem of long relaxation times a *multiple time step* method has been employed to integrate the equations of motion, formulated according to the rRESPA (reversible REference System Propagator Algorithm) scheme. This has allowed us to perform equilibrium MD simulations of PE melts as long as C_{250} for times up to 250 ns.
- The second approach involves nonequilibrium MD of *preoriented configurations*, sampled during EBMC simulations with non-zero field values. The field **α** is removed and the system is left to return to the field-free, equilibrium state, characterized by the absence of any structural anisotropy. The relaxation process is monitored by employing the MD technique in the $NTL_x\sigma_{yy}\sigma_{zz}$ statistical ensemble [Harmandaris *et al.,* 2000], simulating the experiment of *stress relaxation upon cessation of steady-state uniaxial elongational flow.*

Stage III: In this stage, the results of the equilibrium NVT or non-equilibrium $NTL_x\sigma_{yy}\sigma_{zz}$ MD simulations are mapped onto analytical expressions obtained by invoking a mesoscopic theoretical model. For unentangled polymer melts, this is the Rouse model; for entangled melts, this is the reptation model. In the latter case, a mapping of the atomistic chains onto primitive paths needs to be implemented [Kröger *et al.*, 2001].

Results will be presented for the: a) self-diffusion coefficient, b) zero-shear rate viscosity, c) monomer friction factor, and d) spectrum of relaxation times, of PE melts of mean molecular length ranging from C_{78} to C_{250} [Harmandaris *et al.,* 2001]. The results are found to be in excellent agreement with available experimental data, and provide for the first time convincing evidence for the crossover from a Rouse to a reptation-like regime when the molecular length of the PE melts exceeds a value close to about C_{156}.

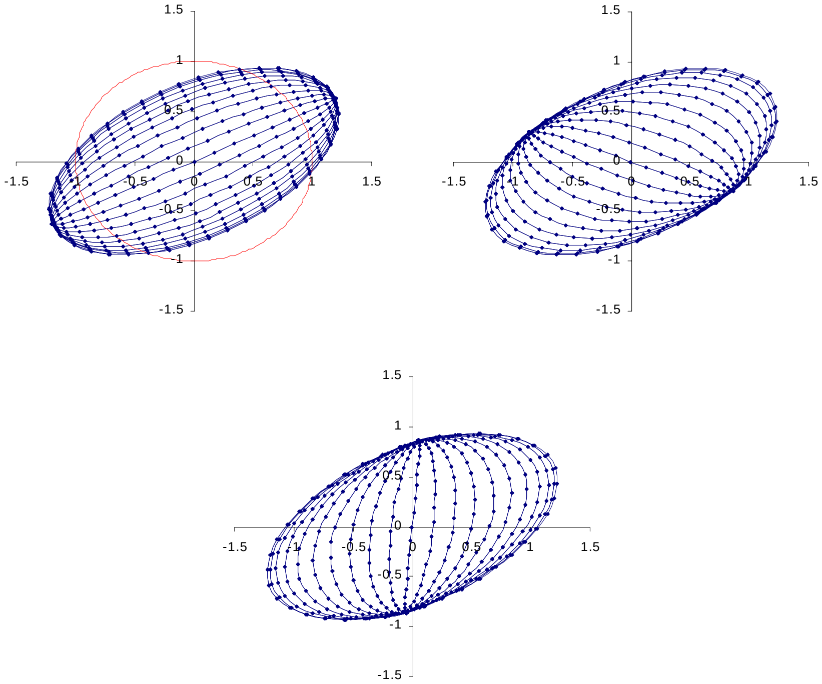
POSTERS

MECHANICAL PROPERTIES AND BEHAVIOR OF CAPSULES IN 3D FLOWS

E. LAC [1], N. A. PELEKASIS [2], J. A. TSAMOPOULOS[2], D. BARTHÈS-BIESEL [1]

[1] CNRS UMR 6600, Université de Technologie de Compiègne, France
[2] Department of Chemical Engineering, University of Patras.

Capsules are composite particles consisting of an internal liquid medium that is enclosed in a deformable membrane. They are frequently met in nature and in industry. In order to evaluate their suitability for a given application or to control their break-up, one must be able to predict their behaviour in flow. An initially ellipsoidal capsule freely suspended in simple shear flow is considered here. The suspending and the internal fluids are supposed to be Newtonian. The analysis of the motion and deformation of the capsule involves resolution of two fluid mechanics problems (flow of the internal and external fluids) coupled with a solid mechanics problem (deformation of the interfacial membrane). Owing to the small dimensions of the capsule, the associated Reynolds number is very small so that Stokes equations apply in both fluids. The aim of the presented work is to determine the influence of different constitutive laws of the membrane on the global response of the capsule. We use the boundary integral method to compute the tensions, the elastic stresses and the velocity of the interface. The mean surface of the membrane is interpolated with bi-cubic B-splines and the integrals are calculated by means of the Gauss quadrature. The case of equal viscosity of the internal and external fluids, in conjunction with a hyperelastic membrane, is first examined. Thus, for a given shear rate we obtain the response of the capsule in terms of the evolution with time of its global deformation and inclination angle. When steady shape is reached, we observe a rotating motion of the capsule known as "tank treading" motion.



Tank treading motion of an initially spherical capsule in shear flow.

MODELING OF VISCOUS EFFECTS IN BLADE COATING FLOWS

E. MITSOULIS, G. ATHANASOPOULOS

Dept. of Mining Eng. & Metallurgy, National Technical University of Athens, GREECE

Previous [1] and new [2] experiments in blade coating flows show the presence of a huge vortex upstream of the blade. Numerical simulations have been undertaken for these geometries and for coating fluids that are purely viscous. The rheological constitutive equation employed is the shear-thinning Carreau model that fits well the shear viscosity of the polymer solutions used as coating fluids. Realistic upstream boundary conditions take into effect the full reservoir and its walls, thus bringing the simulations closer to the experimental findings.

The numerical results show the extent and intensity of the upstream vortex in the reservoir, which is higher for Newtonian fluids and becomes smaller as the shear-thinning character of the fluid becomes more evident. The coating thickness is not affected much by the upstream kinematics but is more affected by the rheology (shear-thinning) and the geometry of the blade. Shear-thinning increases the coating thickness for a given geometry up to power-law index $n > 0.3$, after which a reduction is observed. This new finding is in agreement with previous findings in other geometries for highly shear-thinning fluids. The vortex decreases in size and intensity monotonically and linearly with n, in the range $1 \geq n > 0$. The simulations also provide a wealth of information regarding stresses and pressures and show that some geometries are better than others in coating operations.

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FLUID FLOW AND HEAT TRANSFER DURING LIQUID ENCAPSULATED CZOCHRALSKI CRYSTAL GROWTH OF III-V COMPOUND SEMICONDUCTORS

A. HARKATI*, M. DRIR*, D. OUADJAOUT, R. YOUNSI*****

Theoretical physics laboratory, Physics Institute, USTHB
B.P. 32, El-Alia, 16111 Algiers, (Algeria)
Simulation's laboratory, UDTS, 2 Bd Frantz Fanon, Alger Gare, Algiers, (Algeria)
Fluids Mechanic laboratory, Physics Institute, USTHB
B.P. 32, El-Alia, 16111 Algiers, (Algeria)

Liquid Encapsulated Czochralski (LEC) is frequently used to grow semiconductors compound single crystals. It is another configuration of Czochralski technique. The molten compound is covered with a layer of immiscible liquid in order to avoid the evaporation of volatile component. Thermal and surface tension gradients generates convective motion which affect the quality of the growing crystal. From solving LEC model, we can evaluate the beneficial of harmful effects of the convection on the grown process. The LEC model developed in this investigation is an extension of our precious CZ model. We solve the axisymmetric Navier-Stokes and energy equations, with the Boussinesq approximation coupled with the conduction equation in the crystal. The set of the governing equations are described by means of finite volume procedure, thus the simpler algorithm is used.

NUMERICAL SIMULATION OF HEAT AND MASS TRANSFER IN TRAPEZOIDAL POROUS CAVITY

R. YOUNSI[1], A. HARKATI[2], D. KALACHE[1]

[1]Fluids Mechanic Laboratory, Physics Institute, USTHB
B.P. 32, El-Alia, 16111 Algiers, (Algeria), Fax: (213-21) 24-73-44
[2]Theoretical Physics Laboratory, Physics Institute, USTHB
B.P. 32, El-Alia, 16111 Algiers, (Algeria), Fax: (213-21) 24-73-44

Numerical simulations are conducted for two-dimensional steady state double diffusive flow in a trapezoidal porous cavity. Both the temperature and solute gradients are imposed horizontally, and the two buoyancy effects can either augments or counteract each other. The porous medium in modelled accoeding to the Darcy-Brinkman and Forchheimer model, and the SIMPLER algorithm, based on finite volume approach is used to solving the pressure-velocity coupling. An extensive series of numerical simulations is conducted in the range: $10^3 \leq Gr\ 10^6$, $10^{-8} \leq Da \leq 1, -20 \leq N \leq 20$ and $1 \leq Le \leq 10^2$. It is shown that the main effect of presence of the porous layer is to reduce the heat and mass transfer when the permeability is reduced. With appropriate combination of Grashof number, Lewis number and the buoyancy ratio, multiple cells flow patterns are illustrated.

Key words: Double diffusion, Porous media, Heat and mass transfer, Trapezoidal cavity, Finite volume.

NUMERICAL SIMULATION OF BLOOD FLOW THROUGH STENOTIC ARTERY

L. ACHAB, S. BENHADID

Laboratoire de Rhéologie – Institut de Physique –
Université des Sciences et de la Technologie Houri Boumedienne.
B.P. 32 Bad-Ezzouar 16111. Alger-Algérie.
Fax: (02) 24-73-44

Numerical simulation of blood flow through arterial systems, in particular through arterial stenosis, has been of special interest in recent years because of the information of the local flow pattern that can be provided.

In this present study, the finite element method with the penalty function formulation is applied to simulate two dimensional, time dependent, incompessible, viscous, laminar flow in an axisymetric stenosis.

The equations describing the motions of fluid are those of Navier-Stokes, considered within the velocity-pressure formulation. Penalization of the continuity is implemented by means of the reduced integration technique this eliminating the pressure unknown from the system of equation to be solved. The velocity profile and streamfunctions are presented and discussed in the case of stenosis for different values of Reynolds numbers.

Keywords: Navier-Stokes equations, finite element method, penalization, arterial stenosis.

ANALYTIC SOLUTION FOR THE ANALYSIS OF FLOW IN AN ELASTIC ARTERY

F. IACHACHENE, S. BENHADID

Institut de physique, Laboratoire de Rhéologie, USTHB, Algérie
Fax: (02) 24-73-44

Pulse propagation phenomena in arteries are caused by the interaction of blood with the elastic arterial wall. Therefore, the mathematical statement of the problem should include equations which govern the motion of blood and the motion of arterial wall, and also the relations (boundary conditions) which connect these two motions with each other. This set of equations and conditions make an interesting boundary-value problem.

In this paper, an approximate solution is presented to the problem as function of pressure gradient and the varying radius of the conduct, for weak Reynolds and Womersey numbers. This formulation permit us to get axial and radial velocities along of elastic artery. The velocity fields and wall shear stress are illustrated and discussed in the case of stenosis, aneurysm and along the elastic tube.

Keywords: arterial stenosis, aneurysm, unsteady flow, elastic tube, womersley number.

RHEOLOGICAL PROPERTIES OF HETEROTELECHELIC POLYELECTROLYTES IN AQUEOUS MEDIA

I. KATSAMPAS, C. TSITSILIANIS

Department of Chemical Engineering, University of Patras, 26500 Patras, Greece
and Institute of Chemical Engineering and High – Temperature Chemical Processes, ICE/HT – FORTH,
P.O.Box 1414, 26500 Patras, Greece

We study the rheological properties of physical gels formed in aqueous media from polyelectrolytes, end – capped with short hydrophobic blocks (stickers) of different nature, named heterotelechelic polyelectrolytes. These triblock copolymers (ABC type) are constituted from a long poly(sodium acrylate) chain (PANa) bearing a short chain of polystyrene (PS) at the one end, and poly(n – butyl methacrylate) (PnBMA) at the other end. These copolymers were synthesized by sequential anionic polymerization and modification of the poly(tert – butyl acrylate) middle block by selective hydrolysis and neutralization to its ionic functions. The rheological behavior of the PS – PANa – PnBMA aqueous solutions was explored by steady state and oscillatory shear flow measurements. In steady shear the polymer solutions exhibit extremely high values at low shear viscosity (6 orders of magnitude higher than the viscosity of the media), even for low concentrations (c ~ 0.3%). We also observe a particular rheological behavior, which is characterized from yield stress, several thinning regimes and reversibility at low concentrations. This behavior is attributed to the formation of a transient network constituted from PS and/or PnBMA physical cross – links interconnected by stretched polyelectrolyte chains. From the oscillatory shear measurements we also observed that G'exceeds G'' by about 1 order of magnitude and is independent of ω, indicating that the solution behaves like a highly elastic gel. An unusual observation is that the viscosity of the system seems to be invariant over a wide temperature range (20 – 65 ^{0}C). Finally, the influence of the macromolecular architecture on the rheological properties has been investigated. The length of the middle polyelectrolyte chain, the degree of ionization, the nature and the length of the end – blocks play a significant role in the rheological properties.

TEMPERATURE AND SHEAR INDUCED THICKENING PROPERTIES OF AQUEOUS SOLUTIONS OF N-ISOPROPYLACRYLAMIDE-BASED POLYMERS

G. BOKIAS[1], Y. MYLONAS[1], G. STAIKOS[1],
D. HOURDET[2], I. ILIOPOULOS[2], G.G. BUMBU[3], C. VASILE[3]

[1]Department of Chemical Engineering, University of Patras, GR-26500 Patras, Greece
[2]LABORATOIRE DE PHYSICO-CHIMIE MACROMOLÉCULAIRE UMR 7615, ESPCI-CNRS-UPMC, 10 RUE VAUQUELIN, 75231 PARIS CEDEX 05, FRANCE
[3]"P.Poni" Institute of Macromolecular Chemistry, 41A Gr. Ghica Voda Alley, Ro.6600 IASI, Romania

Poly(N-isopropylacrylamide), PNIPAM, is a water-soluble polymer, extensively studied during the last fifteen years mainly due to its Lower Critical Solution Temperature (LCST) behavior in water. As a result of the delicate hydrophilic-hydrophobic balance arising from the chemical structure of N-isopropylacrylamide (NIPAM), PNIPAM phase separates from aqueous solution as temperature increases above 32-33°C. Based on this property, interesting stimuli-responsive rheological properties can be obtained by properly designing NIPAM-based copolymers able to maintain a strong tendency to form hydrophobic microdomains in aqueous solution as temperature increases, while avoiding macroscopic phase separation.

An example offer the graft copolymers consisting of a hydrophilic backbone, like carboxymethylcellulose or random (acrylic acid) - (2-acrylamido-2-methyl-1-propanesulphonic acid) copolymers, and PNIPAM side chains. In semi-dilute aqueous solution, hydrophobic aggregation of the PNIPAM chains above LCST lead to a pronounced temperature-induced viscosity enhancement, explained by theformation of a physical network. These thickening properties are very shear-sensitive and an important shear thinning is observed, because the physical crosslinks, stabilized by the relatively weak hydrophobic interactions, break under flow.

The opposite, shear-induced thickening behaviour, can also be observed if we use a different structure of NIPAM-containing derivatives. Such copolymers are based on a NIPAM-backbone, hydrophobically modified with a relatively large number of charged dodecyl- or octadecyl- groups. At low shear rate in semi-dilute aqueous solution these strong hydrophobic groups form mainly intrachain aggregates and the solution viscosity is very low. When shear is applied, these aggregates are deformed and above a critical shear rate interchain hydrophobic junctions are formed. As a result, an original sol/gel transition occurs at the critical shear rate. The sharpness of this shear-induced thickening phenomenon and the critical shear rate depend on various factors: length of the alkyl groups, alkyl content, polymer concentration and temperature.

STEADY-STATE FULLY-DEVELOPED TWO-PHASE FLOW IN POROUS MEDIA: MECHANISTIC MODEL AND A CONJECTURE CONCERNING THE UNDERLINE PRINCIPLE

M.S. VALAVANIDES*, A.C. PAYATAKES**

**ICEHT/FORTH, Department of Chemical Engineering, University of Patras
*IRC Help-Forward/FORTH, Fax: +3061 990328

A recently developed predictive model (DeProF) considers steady-state two-phase flow in porous media (SS2φPM) as a composition of three-experimentally observed- flow patterns, namely CPF (connected-oil pathway flow) GD (ganglion dynamics) and DTF (drop traffic flow). The key difference between these prototype flow patterns is the degree of disconnection of the non-wetting phase ('oil') which, in turn, affects the relative magnitude of the rate of energy dissipation caused by capillary effects compared to that caused by viscous stresses. The observed flow is usually a mixture of the basic prototype flows. Each flow pattern prevails over mesoscopic-scale regions of the porous medium (ranging from a few to several hundred pores), whereas the macroscopic flow is homogeneous.

Analytical functions that incorporate all the basic pore scale flow mechanisms are derived for each prototype flow. Disconnected-oil flow is 'homogenized' at the unit cell level, yielding a hydraulic conductance that is a function of the local pore geometry, the local flow arrangement, and the local flow velocity. The length-scale gap between micro- and macroscopic flow is bridged using EMT (effective medium theory). Then, all physically admissible (internally constrained) combinations of the prototype flows are determined. Postulating that each physically admissible flow combination has the same probability of being 'visited', we can evaluate the mean macroscopic relative contribution of each pattern to the total flow, as well as the 'expected' flow arrangement, flowrates and power dissipation. The new model accounts for the non-linearity of the flow as well as for the effects of all the system parameters. The quantitative and qualitative agreement between existing sets of data and the corresponding theoretical predictions of the new model is excellent.

In order further to exploit the predictive capability of the DeProF model, several macroscopic interstitial physical quantities corresponding to each prototype flow, as well as to the total flow, are determined. These quantities are: the magnitude of the domain of physically admissible solutions, the interfacial area per unit volume, the mechanical power dissipation per unit volume, and the degree of disconnectedness of the non-wetting phase. The dependence of these characteristic quantities on the values of the flow system parameters is presented in graph form.

We make the following *conjecture*: The system under consideration is far from equilibrium and is kept at this condition through the continual injection of mass and mechanical energy. The mixture of the various dissipative prototype flows that is established for each set of system parameters values is decided through a dialectic between the energy of the system and the entropy of the system. This conjecture may lead to the *proper* macroscopic phenomenological description of two-phase flow in porous media.

NON-NEWTONIAN BEHAVIOR FLOW THROUGH ARTERIAL STENOSIS

L. ACHAB, S. BENHADID

Laboratoire de Rhéologie – Institut de Physique –
Université des Sciences et de la Technologie Houri Boumedienne.
B.P. 32 Bad-Ezzouar 16111. Alger-Algérie.
Fax: (02) 24-73-44

It is clear that the non-Newtonian behavior of the blood, as well as local flow patterne, play an important role in the genesis and development of the stenosis, in arterial systems, which is one of the most frequently occuring abnormalities in man.
In this work, we study analytically the influence of the rheological parameters blood, and geometrical effects of the stenosis of hydrodynamics factors essentially on the pressire drop, flow resistance (or impedance) and wall shear stress. Restricting our attention to fluids of the generalized Newtonian class, i.e., non-Newtonian fluids exhibiting a yield stress. The analysis is carried out for the HERSCHEL-BULKLEY and ROBERTSON STIFF rheological models. Results illustrated for a moderated size stenosis, have allowed a comparison between the behavior of Newtonian and non-Newtonian blood.

VISCOELASTIC FLOW BEHAVIOR OF A SIDE-CHAIN NEMATIC LC POLYACRYLATE

[1]L. HILLIOU, [1]A.G. FEIO, [1]A. F. MARTINS, [2]D. COLLIN, [2]P. MARTINOTY

[1]Dept. Ciência dos Materiais, Faculdade de Ciências e Tecnologia,
Universidade Nova de Lisboa, 2825-114 Caparica, Portugal
[2]Lab. Dynamique des Fluides Complexes, Unité Mixte de Recherche ULP-CNRS nº7506,
4 rue Blaise Pascal, 67070 Strasbourg Cedex, France

The viscoelastic properties of a side-chain nematic polyacrylate (SCNP) have been investigated by means of microrheology experiments, conducted as a function of temperature and sample thickness, and rheo-NMR experiments. Microrheology experiments evidenced a transition from a liquid-like behaviour to a solid-like behaviour as the temperature is lowered. This result is in harmony with rheo-NMR experiments, which show that the reorientation behaviour of the SCNP following the application of a step rotation to the sample, under the magnetic field of the NMR spectrometer, strongly depends on temperature and thermal history. The change in the viscoelastic behaviour is related to the development with time of a mesoscopic structure, which vanishes at high temperature. Simulations of experimental NMR spectra were performed in order to assess the time evolution of the orientational distribution of the nematic side-chains, during the reorientation process. This analysis allows for a qualitative description of the complex reorientation behaviour of the SCNP.

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STATIC AND DYNAMIC FILTRATION PROPERTIES OF POLYMERS IN WATER-BASED DRILLINNG MUDS

N. KHERFELLAH[1], K. BEKKOUR[2], S. HAMZA[1], M. KHODJA[1], S. BENHADID[3]

[1]Centre de Rechereche et Développement (SONATRACH), 1 Avenue du 1er Novembre 35000
Boumerdes, ALGERIE
[2]Institut de Mécanique des Fluides, UNR 7507 ULP-CNRS. 2, rue Boussingault
67000 Strasbourg, FRANCE
[3]Université de Sciences et de la Technologie Houari Boumediène
Institut de Physique, Laboratoire de Rhéologie, BP 32 El Alia, ALGERIE

Deep well drilling require the development of drilling fluid formulations adapted to high formation temperatures: a major cause of problems is the thermal degradation of chemical additives used in water based formulations that often occurs while drilling high temperature and pressure wells. Such a degradation can lead to strong variations in rheological and filtration control for the fluid system. The filtration control polymers are sufficiently flexible and deformable to fill the small irregular pore openings of the final particle bridge thus provide positive leak-off control for the fluid.

A laboratory study has been undertaken to elucidate the influence of structural parameters of polymer / electrolyte systems commonly used for the formulation of saturated salt water-based muds on their performance as filtrate reducers or viscosifiers.

The dependence of rheological properties of water based mud using polymer additives on polymer molecular characteristics has been studied. The additive structure and molecular weight were selected in order to limit the damage due the filtrate invasion. The approach was validated on long core filtration test performed under representative reservoir conditions.

The results indicate that polymer dimensions which depend on both salinity and polymer molecular weight have a major influence on the efficiency in inhibiting cuttings dispersion.

Filtration properties of the investigated model fluids have been found to be strongly dependent on polymer / salt interactions.

Key words: Polymers, Flow, Dynamic, Rheology, Porous media, Colloid

SLOW FLOWS OF A NON-NEWTONIAN DROP IN A NON-NEWTONIAN FLUID

FRANCESCO GRECO

Institute for the Technology of Composite Materials (ITMC), CNR
and
Chemical Engineering Department, University of Naples "Federico II"
P.le Tecchio 80, 80125 Naples, ITALY

The fluid dynamics of a single drop immersed in an immiscible fluid in motion received much attention in the rheological literature. Indeed, the study of such an idealized problem is directly relevant in dilute systems as the starting point to obtain rheological predictions concerning the system as a whole. It has to be recalled in this respect that even when the two component fluids are Newtonian, the total fluid is non-Newtonian, because of the elastic effects associated with the presence of an interface.

In the single drop fluid dynamics, a part of the boundary conditions to be satisfied is assigned on the surface of the deforming drop, which is itself unknown. This is a free boundary problem, where the intrinsic nonlinearities lead to an apparently insoluble mathematics. A perturbation approach, i.e., considering the limit of small deformations "around" the spherical reference shape, seems to be the only available route to analytical results.

In this work, the component fluids are taken to be second-order fluids. Their constitutive properties (viscosities, and normal stress difference coefficients), together with the interface properties (an interfacial tension), generate two nondimensional quantities mainly governing single drop deformation: i) the ratio of viscous to interfacial stresses, the so-called capillary number Ca, and ii) the ratio N of normal to interfacial stresses. Conditions of small Ca and N are seen to correspond to small drop deformations from the unperturbed spherical shape, because interfacial forces are dominant. In these conditions, which surely hold for sufficiently slow flows, it is then possible to adopt a perturbation procedure in the fluidodynamic problem, with capillary number Ca and N as the expansion parameters.

In the presentation, we will illustrate the perturbative calculations and the results, especially pointing out the fluid elasticities effects, which are new with respect to the Newtonian case. We will also indicate some future directions of work on the experimental side, giving suggestions for designing experiments directly testing the theory.

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