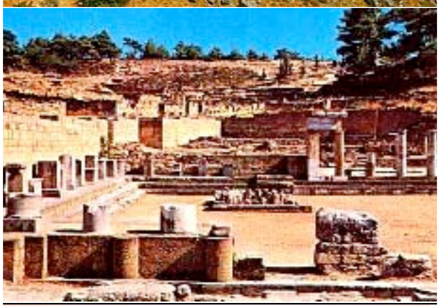

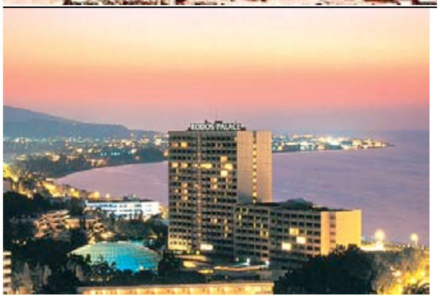

HSR 2007

HELLENIC SOCIETY OF RHEOLOGY

Rhodes, Greece

June 5-10, 2007

BOOK OF ABSTRACTS

CHAIRS' MESSAGE

It is with great pleasure that we welcome all delegates and accompanying persons to the 5th Meeting of the Hellenic Society of Rheology, HSR 2007, in Rhodes, Greece. HSR meetings are rotated every 3 years among various locations around Greece and Cyprus. This is the 5th meeting since the foundation of the Society in 1996, when its 1st meeting was held in Nicosia, Cyprus. The 2nd meeting was held in 1998 in Herakleion, Crete, the 3rd meeting in 2001 in Patras, and the 4th meeting in 2004 in Athens. Rhodes has been chosen for this meeting, as it is the capital of Dodecanese Islands, and boasts many historic sites as well as sun, sea, excellent facilities, etc., and it has been a place of tourism and holidays since antiquity.

The HSR 2007 Meeting is a very special meeting as it is combined with the XVth International Workshop on Numerical Methods for Non-Newtonian Flows (XVth IWNMNNF). The HSR meeting starts with sessions on experimental rheology and rheometry and continues with computational rheology, where many Greek rheologists contribute. The combined Conference includes 2 plenary and 55 oral lectures and 10 posters. The scientific papers will be presented under 8 major themes. We hope that this Conference will promote and facilitate scientific exchange, collaboration and interactions between participants as well as their organisations in advancing science and technology based on rheology.

Rhodes is reputed as the "Island of the Sun" and boasts some terrific beaches together with ancient and medieval sights that attract people from around the world. We hope all international delegates will experience the important attractions that Rhodes has to offer during their stay on the island.

We thank all the sponsors of this Meeting for their generous support. We are indebted to the members of the Organising and Scientific Committees and other individuals for their commitment and hard work in order to make this Meeting a successful event.

Prof. Evan Mitsoulis
Conference Chair

Prof. Vlasis Mavrantzas
Conference Vice-Chair

Table of Contents

HSR 2007 Organising Committee

E. Mitsoulis (Chair), Athens
V. Mavrantzas (Co-Chair), Patras
A. Payatakes, Patras
N. Pelekasis, Volos
D. Theodorou, Athens
J. Tsamopoulos, Patras
Ch. Tsenoglou, Athens
D. Vlassopoulos, Herakleion

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D. Theodorou, Greece
J. Tsamopoulos, Greece
Ch. Tsenoglou, Greece
D. Vlassopoulos, Greece

HELLENIC SOCIETY OF RHEOLOGY

The ***Hellenic Society of Rheology (HSR)*** was officially formed on June 16th, 1996, in Athens, Greece, by the Greek judicial authorities having the necessary core of the first 20 founding members. 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.

Rheology enters in some form into almost every study of material properties. Many physicists, chemists, engineers, biologists and mathematicians find a common meeting ground in the Society's meetings and publications. It is a small society compared to many others, membership currently being about 40. Membership in HSR is open to all researchers in the field, and to all persons who feel the activities of the Society advance their professional development. The membership represents a wide spectrum of individuals from academic, industrial, and governmental institutions whose activities include both phenomenological and molecular theories, instrumentation, the study of many types of materials such as polymers, metals, petroleum products, rubber, paint, printing ink, ceramics and glass, foods, biological materials, floor preparations and cosmetics, and a wide range of practical applications.

The Hellenic Society of Rheology is one of the fifteen (15) founding members of the *European Society of Rheology*. By virtue of this affiliation, all Members of the Society receive the ESR's Newsletter. The Society is also a member of the International Committee on Rheology, which organizes the *International Congress on Rheology*, held every four years.

Please visit the HSR website at:

http://esperia.iesl.forth.gr/~hsr/HSR.html

HSR Executive Committee (2006-2008)

President	A. Alexandrou
President-Elect	A. Gotsis
Secretary/Treasurer	S.G. Hatzikiriakos
President-Past	V. Mavrantzas
Members-at-large	E. Mitsoulis
	Ch. Tsenoglou
Webmaster	A. Gotsis

HSR 2007 Program Summary

Tuesday, June 5, 2007

17:00-19:00 *Registration, Hotel Rodos Palace*
20:30-22:30 *Cocktail Party by the Hotel Rodos Palace Pool*

Wednesday, June 6, 2007

08:00-08:30 *Registration for HSR*
08:30-08:40 *Welcome remarks for HSR*
08:40-09:20 **Plenary presentation by Prof. Dimitris Vlassopoulos**
09:25-10:15 **2 presentations**
10:15-10:45 *Coffee break*
10:45-11:35 **2 presentations**
11:35-11:55 *Discussion*
12:00-14:00 *Lunch*

14:00-18:00 *Free time*

18:00-18:30 *Registration for Workshop*
18:30-18:40 *Welcome remarks – Motivation – Organizational details*
18:40-19:20 **Plenary presentation by Prof. Roger Tanner**
19:25-21:00 **4 presentations**
21:00-22:30 *Welcome Buffet*

Thursday, June 7, 2007

08:00-10:00 **5 presentations**
10:05-10:20 *Coffee break*
10:20-12:00 **4 presentations (1 from HSR)**
12:05-14:00 *Lunch*
14:00-15:35 **4 presentations (3 from HSR)**
15:40-15:55 *Coffee break*
15:55-16:15 **2 presentations (1 from HSR)**
17:00 *Free Evening*

Friday, June 8, 2007

08:00-10:00 **5 presentations (2 from HSR)**
10:05-10:20 *Coffee break*
10:20-12:00 **4 presentations (1 from HSR)**
12:05-14:00 *Lunch*
14:00-15:35 **Poster Session – 10 posters (7 from HSR)**
15:40-15:55 *Coffee break*
16:00-20:30 *Excursion to Lindos*

Saturday, June 9, 2007

08:00-10:00 **5 presentations (1 from HSR)**
10:05-10:20 *Coffee break*
10:20-12:00 **4 presentations (1 from HSR)**

12:05-14:00 *Lunch*

14:00-15:35 **4 presentations**

15:40-15:55 *Coffee break*

15:55-16:15 **2 presentations**

16:45-20:30 *Free Evening*

20:30-22:30 *Conference Dinner*

Sunday, June 10, 2007

09:00-10:35 **4 presentations (2 from HSR)**

10:35-11:00 *Coffee break*

11:00-11:20 **1 presentation**

11:25-11:55 **Discussion – Closing Remarks**

12:00-14:00 *Lunch*

End of Workshop

Total:

1 Plenary presentation by Prof. D. Vlassopoulos (45 min)

1 Plenary presentation by Prof. R. Tanner (45 min)

55 oral presentations (16 from HSR) (25 minutes each)

10 Posters (7 from HSR)

Day 1: Wednesday Morning, June 6, 2007

08:00-08:30 *Registration*
08:30-08:40 Welcome remarks – Motivation – Organizational details
Evan Mitsoulis, National Technical University of Athens, Greece

Plenary Lecture

Chair: E. Mitsoulis

08:40-09:20 **(A83) Yielding mechanisms in colloidal glasses**
Dimitris Vlassopoulos, G. Petekidis, FORTH & University of Crete, Herakleion, Greece
M.E. Helgeson, N.J. Wagner, University of Delaware, USA
S. Rogers, P. Callaghan, Victoria University, Wellington, New Zealand

Session 1: Experimental Rheology

Chair: V.G. Mavrantzas

09:25-09:45 **(A40a) Rheology and microscopic rearrangements of colloidal glasses and shear-induced crystals**
N. Koumakis, G. Petekidis, FORTH & University of Crete, Herakleion, Greece

09:50-10:10 **(A40b) Rheology of attractive hard sphere glasses and gels**
N. Koumakis, G. Petekidis, D. Vlassopoulos, FORTH & University of Crete, Herakleion, Greece
K.N. Pham, S.U. Egelhaaf, W.C.K. Poon, P.N. Pusey, University of Edinburgh, UK

10:15-10:45 *Coffee break*

10:45-11:05 **(A84) Ageing and yielding in a soft colloidal glass**
C. Christopoulou, G. Petekidis, D. Vlassopoulos, FORTH & University of Crete, Herakleion, Greece

11:10-11:30 **(A80) Rheological characterization of foodstuff used in rolling experiments and modeling via integral constitutive equations**
E. Muliawan, S.G. Hatzikiriakos, University of British Columbia, Vancouver, Canada
S. Sofou and E. Mitsoulis, National Technical University of Athens, Greece

11:35-11:55 *Discussion*

12:10-14:00 *Lunch*

In Bold letters are contributions from HSR members

Day 1: Wednesday Evening, June 6, 2007

18:00-18:30 *Registration*
18:30-18:40 Welcome remarks – Motivation – Organizational details
Evan Mitsoulis, National Technical University of Athens, Greece

Plenary Lecture
Chair: E. Mitsoulis

18:40-19:20 The changing face of computational rheology
Roger Tanner, University of Sydney, Sydney, NSW, Australia

Session 1: Viscoelastic Suspensions
Chair: B. Khomami

19:25-19:45 (A24) Rigid rods in non-homogeneous shear flow
M.J. Green, R.C. Armstrong, MIT, Cambridge, MA, USA
R.A. Brown, Boston University, Boston, MA, USA

19:50-20:10 (A30) Numerical simulations of concentrated viscoelastic suspensions in an elongational flow
G. D'Avino, P.L. Maffetone, University of Napoli, Italy
M.A. Hulsen, G.W.M. Peters, Eindhoven University of Technology, The Netherlands

20:15-20:35 (A23) Numerical simulation of polymer melts containing short and long fibers
P. Wapperom, D.G. Baird, G. Velez, A.P.R. Eberle, Virginia Tech, Blacksburg, VA, USA

20:40-21:00 (A70) Numerical simulation of suspensions of rigid and deformable particles in polymer melts
Ahamadi Malidi, O.G. Harlen, University of Leeds, UK

21:05-22:30 *Welcome buffet – Registration (cont.)*

In Bold letters are contributions from HSR members

Day 2: Thursday Morning, June 7, 2007

Session 2: Multiscale Modeling and Molecular Simulations

Chair: V.G. Mavrantzas

8:00-8:20 (A45) Realizing rheological dreams: efficient solution of highly dimensional Fokker-Planck equations
A. Ammar, Laboratoire de Rheologie, Grenoble, France
F. Chinesta, ENSAM, Paris, France
R. Keunings, Université Catholique de Louvain, Louvain-la-Neuve, Belgium

8:25-8:45 (A20) Optimal choices of correlation operators in Brownian simulation methods
Raz Kupferman and Yossi Shamai, The Hebrew University, Jerusalem, Israel

8:50-9:10 (A9) A log transformation applied to the method of Brownian configuration fields
Claude Mangoubi, and Raz Kupferman, The Hebrew University, Jerusalem, Israel
Martien A. Hulsen, Eindhoven University of Technology, The Netherlands

9:15-9:35 (A11) A P3M method for computation of many-body hydrodynamic interactions in a confined geometry: application to migration and apparent slip in nondilute polymer solutions
J.P. Hernandez-Ortiz, S. Anekal, M.D. Graham, University of Wisconsin-Madison, USA

9:40-10:00 (A78) Frictional drag properties of polymeric solution in complex kinematics flows: a multi-scale simulation approach
A.P. Koppol, R. Sureshkumar, Washington University, St. Louis, MO, USA
B. Khomami, University of Tennessee, Knoxville, TN, USA

10:05-10:20 *Coffee break*

Session 3: Multiscale Modeling and Molecular Simulations (Cont'd)

Chair: R. Keunings

10:20-10:40 (A34) DPD as a tool for rheological characterization
T.F. Clarke and R.C. Armstrong, MIT, Cambridge, MA, USA

10:45-11:05 (A73) Atomistic Monte-Carlo simulation of a polymer melt under a flow field by employing generalized ensembles
Chunggu Baig and V.G. Mavrantzas, University of Patras, Greece; FORTH-ICE/HT, Patras, Greece

11:10-11:30 (A6) Rheological and Entanglement Characteristics of Linear Chain Polyethylene Liquids in Planar Couette and Planar Elongational Flows
J.M. Kim, D.J. Keffer, B.J. Edwards, University of Tennessee, USA
M. Kroeger, ETH, Zurich, Switzerland

11:35-12:00 (A42) Transient 3D Flow of Polymer Solutions
N.F. Morrison, J.M. Rallison, University of Cambridge, UK

12:05-14:00 *Lunch*

In Bold letters are contributions from HSR members

Day 2: Thursday Afternoon, June 7, 2007

Session 4: Viscoplastic Fluids – Modeling and Simulations

Chair: A.N. Beris

14:00-14:20 **(A49) Steady bubble rise and deformation in Bingham fluids and conditions for their entrapment**
J. Tsamopoulos, Y. Dimakopoulos, N. Chatzidai, G. Karapetsas, M. Pavlidis, University of Patras, Greece

14:25-14:45 **(A76) Weakly compressible Poiseuille flows of a Bingham fluid**
E. Taliadorou, G. Georgiou, A. Alexandrou, University of Cyprus, Nicosia, Cyprus

14:50-15:10 **(A79) Numerical simulation of calendering of viscoplastic materials**
E. Mitsoulis, S. Sofou, National Technical University of Athens, Greece

15:15-15:35 (A59) Wave evolution in two-layer pressure driven flow – Newtonian upper layer over a non-Newtonian bottom layer
P. Valluri, P.D.M. Spelt, O.K. Matar, C.J. Lawrence, Imperial College London, UK

15:40-15:55 *Coffee break*

15:55-16:15 **(A85) Squeeze flow of carbopol gels**
E. Mitsoulis, I. Argyropaidas, National Technical University of Athens, Greece

16:20-16:40 (A63) Blood hemodynamics in carotid bifurcation: influence of rheological models
P. Ternik, Z. Zunic, J. Marn, University of Maribor, Slovenia

16:45-17:00 Discussion

Free Evening

In Bold letters are contributions from HSR members

Day 3: Friday Morning, June 8, 2007

Session 5: Viscoelastic Flow Instabilities

Chair: P.J. Oliveira

8:00-8:20 (A8) Using Newton-GMRES for viscoelastic flow time-steppers
Z. Anwar and R.C. Armstrong, MIT, Cambridge, MA, USA

8:25-8:45 (A46) On a new elastic instability: bifurcation in a cross-slot
R.J. Poole, University of Liverpool, UK
M.A. Alves, University of Porto, Portugal
P.J. Oliveira, University of Beira Interior, Covilha, Portugal

8:50-9:10 (A72) Bifurcation analysis of flow instabilities in polymer melts during extrusion
M.E. Kavousanakis, C.I. Siettos, A.G. Boudouvis, National Technical University of Athens, Greece
L. Russo, University of Naples, Italy
G. Georgiou, University of Cyprus, Nicosia, Cyprus

9:15-9:35 (A31) Modeling of axisymmetric instabilities observed during the electrospinning of highly conducting, non-Newtonian jets
C.P. Carroll, Y.L. Joo, Cornell University, Ithaca, NY, USA

9:40-10:00 (A53) Cavity filling process modeling by rheological characterization and large scale computation
K. Christodoulou, R. Mehrabi, A. Mehrabi, E. Rozenbaum, Avery Research Center, Pasadena, CA, USA

10:05-10:20 *Coffee break*

Session 6: Viscoelastic Flow Instabilities (Cont'd)

Chair: G.C. Georgiou

10:20-10:40 (A52) A parallel adaptive unstructured finite volume method for linear stability (normal mode) analysis of viscoelastic fluid flows
M. Sahin, H.J. Wilson, University College London, UK

10:45-11:05 (A9) A new stability mechanism associated with the Oldroyd-B model in creeping flow regime
Raz Kupferman, The Hebrew University, Jerusalem, Israel

11:10-11:30 (A54) Coil-stretch transition and the break down of continuum models
M. Bajaj, J. Ravi Prakash, Monash University, Melbourne, Australia
M. Pasquali, Rice University, Houston, TX, USA

11:35-11:55 (A15) On kinetic models for dilute suspensions of rigid rods
F. Otto, University of Bonn, Germany
A. Tzavaras, University of Maryland, MD, USA

12:00-14:00 *Lunch*

In Bold letters are contributions from HSR members

Day 3: Friday Afternoon, June 8, 2007

Session 7: Poster Session

14:00-15:40 **P1. (A74) A generalized single-conformation tensor viscoelastic model based on principles of non-equilibrium thermodynamics**
P. Stefanou, Chunggi Baig, V.G. Mavrantzas, University of Patras, Greece

P2. (A58) Numerical simulation of complex fluid flows with non-Newtonian differential models
O. Wuensch and M. Krebs, University of Kassel, Germany

P3. (A57) Numerical simulations of flow in a variable speed co-rotating twin screw extruder
C. Tzoganakis and S. Zhu, University of Waterloo, Canada
T. Shigeishi and K. Tikara, Japan Steel Works, Hiroshima, Japan

P4. (A48) Correlating the rheology of PVC pastes with particle characteristics
M.G. Rasteiro, L.M. Ferreira, A. Tomàs, S. Figueiredo, University of Coimbra, Portugal

P5. (A80) Rheological characterization of foodstuff used in rolling experiments and modeling via integral constitutive equations
E. Muliawan, S.G. Hatzikiriakos, University of British Columbia, Vancouver, Canada
S. Sofou and E. Mitsoulis, National Technical University of Athens, Greece

P6. (A81) Predicting the behaviour of nylon-6 through industrial spin packs
A. Gustin and A. Zupancic, University of Ljubljana, Slovenia
E. Mitsoulis, National Technical University of Athens, Greece

P7. (A71) Numerical simulation of the extrusion of strongly compressible liquid foams
E. Taliadorou and G. Georgiou, University of Cyprus, Nicosia, Cyprus
E. Mitsoulis, National Technical University of Athens, Greece

P8. (A77) Annular Poiseuille flow of a Newtonian liquid with non-monotonic slip along the walls
M. Chatzimina, G. Georgiou, University of Cyprus, Nicosia, Cyprus
K. Housiadas, University of the Aegean, Samos, Greece
S.G. Hatzikiriakos, University of British Columbia, Vancouver, Canada

P9. (A41a) Comparative study of multi-mode constitutive equations for film blowing process
S. Sarafrazi, F. Sharif, Amirkabir University of Technology, Tehran, Iran

P10. (A82) The temperature dependence of the Rouse mode relaxation spectrum and zero shear rate viscosity in cis-1,4-polybutadiene: results from long atomistic molecular dynamics simulations down to the glass transition temperature Tg
G. Tsolou, V.G. Mavrantzas, University of Patras, Greece

15:40-15:55 *Coffee break*

16:00-20:30 *Excursion to Lindos*

In Bold letters are contributions from HSR members

Day 4: Saturday Morning, June 9, 2007

Session 8: Viscoelastic Fluids - Modeling and Simulations

Chair: J. Tsamopoulos

8:00-8:20 **(A47) On the gas penetration in periodically constricted circular tubes filled with viscoelastic liquids**
Y. Dimakopoulos, J. Tsamopoulos, University of Patras, Greece

8:25-8:45 (A27) The log-conformation tensor approach in the FVM framework: benchmark solutions and stability analysis
A. Afonso, M.A. Alves, University of Porto, Portugal
F.T. Pinho, University of Minho, Braga, Portugal
P.J. Oliveira, University of Beira Interior, Covilha, Portugal

8:50-9:10 (A13) Oscillating channel flows of UCM and Oldroyd-B fluids: numerical and analytical solutions
A.S.R. Duarte, A.I.P. Miranda, P.J. Oliveira, University of Beira Interior, Covilha, Portugal

9:15-9:35 (A39) Numerical simulation of the flow of a PTT fluid past a cylinder
H. Kamal, L. Thais, G. Mompean, H. Naji, Polytech'Lille, France

9:40-10:00 (A84) On the numerical treatment of integral models for elasticity in a compressible fluid
P.C Bollada, T.N. Phillips, Cardiff University, UK

10:05-10:20 *Coffee break*

Session 9: Viscoelastic Fluids - Modeling and Simulations (cont'd)

Chair: E. Mitsoulis

10:20-10:40 **(A51) Viscoelastic analysis of complex flows: from the constitutive model through the numerical simulations and their experimental validation**
I. Sirakov, University of St-Etienne, France
E. Mitsoulis, National Technical University of Athens, Greece

10:45-11:05 (A50) Numerical simulation of viscoelastic flows in cross-slot flow devices
M.F. Webster, F. Belblidia, B. Puangkird, University of Wales, Swansea, UK

11:10-11:30 (A19) Prediction of die swell in polymer melt extrusion using an Arbitrary Lagrangian Eulerian (ALE) based finite element method
V. Ganvir, A. Lele, Pune, India
R. Thaokar, IIT, Bombay, India
B.P. Gautham, NCL, Pune, India

11:35-11:55 (A41b) Non-isothermal simulation of the film-blowing process using the multi-mode extended pom-pom model
S. Sarafrazi, F. Sharif, Amirkabir University of Technology, Tehran, Iran

12:00-14:00 *Lunch*

In Bold letters are contributions from HSR members

Day 4: Saturday Afternoon, June 9, 2007

Session 10: Complex Materials: Experiments and Modeling

Chair: M.F. Webster

14:00-14:20	(A22a) Computing with power-law viscoelastic materials Roger Tanner, F. Qi, S.-C. Dai, University of Sydney, NSW, Australia
14:25-14:45	(A68) Characterization of the compressive behaviour of brain tissue and constitutive modeling G.W.M. Peters, M. Hrapko, J.A.W. van Dommelen, J.S.H.M. Wismans, Eindhoven University of Technology, The Netherlands
14:50-15:10	(A43) Experimental and numerical evaluation of drop deformation and break-up in complex flow fields R.D. Egholm, P. Szabo, Technical University of Denmark, Lyngby, Denmark P. Fischer, ETH, Zurich, Switzerland K. Feigl, Michigan Technological University, Houghton, MI, USA
15:15-15:35	(A67) Experimental and numerical study of cavitation in journal bearings P.C. Bollada, T.N. Phillips, Cardiff University, UK P.R. Williams, R.L. Williams, University of Wales, Swansea, UK
15:40-15:55	*Coffee break*

Session 11: Complex Materials: Experiments and Modeling (Cont'd)

Chair: G.W.M. Peters

15:55-16:15	(A26) Modeling of non-isothermal electrospinning of polymer melts with and without crystallization E. Zhmayev, Y.L. Joo, Cornell University, Ithaca, NY, USA
16:20-16:40	(A37) Structure-property relationships for the Newtonian and the non-Newtonian flow of polymer solutions F. Meyer, H. Storz, J. Storz, A. Bingoel, W.-M. Kulicke, University of Hamburg, Germany
16:45-20:30	*Free time*
20:30-22:30	*Conference dinner*

In Bold letters are contributions from HSR members

Day 5: Sunday Morning, June 10, 2007

Session 12: Turbulence in Complex Fluids

Chair: G. Mompean

9:00-9:20 **(A56) Dynamic K-L analysis of coherent structures based on DNS of turbulent Newtonian and viscoelastic flows**
G. Samanta, A.N. Beris, University of Delaware, Newark, DE, USA
G. Oxberry, MIT, MA, USA
R. Handler, Naval Research Laboratory, Washington, DC, USA
K. Housiadas, University of the Aegean, Samos, Greece

9:25-9:45 **(A55) A log-exponential mapping for the preservation of positive definiteness in the numerical integration of viscoelastic constitutive equations**
K. Housiadas, University of the Aegean, Samos, Greece
L. Wang, A.N. Beris, University of Delaware, Newark, DE, USA

9:50-10:10 (A38) Direct and large eddy numerical simulations of FENE-P drag reduction flows
L. Thais, G. Mompean, Polytech'Lille, France
A.E. Tejada-Martinez, University of South Florida, FL, USA
T.B. Gatski, University of Poitiers, ENSMA, France

10:15-10:35 (A29) A turbulence closure for viscoelastic fluids based on the FENE-P model
F.T. Pinho, University of Minho, Braga, Portugal
P.R. Resende, University of Porto, Portugal
C.F. Li, R. Sureshkumar, Washington University, St. Louis, MO, USA
B.A. Younis, University of California, Davis, CA, USA

10:35-11:00 *Coffee break*

11:00-11:20 (A21) DNS experiments of surfactant drag reducing fluid flows
S. Guillou, R. Makhloufi, F. Hadri, A. Besq, University of Cherbourg, France

11:25-11:55 Discussion – Closing remarks

12:00-14:00 *Lunch*

END OF WORKSHOP

In Bold letters are contributions from HSR members

PLENARY LECTURES

Yielding Mechanisms in Colloidal Glasses

Matthew E. Helgeson [1], Simon Rogers [2], George Petekidis [3,4],
Norman J. Wagner [1], Paul Callaghan [2] and Dimitris Vlassopoulos [3,4]

[1] Department of Chemical Engineering, University of Delaware, USA
[2] Victoria University, Wellington, New Zealand
[3] Institute of Electronic Structure and Laser, Foundation for Research and Technology - Hellas (FORTH), Herakleion, Greece
[4] Department of Materials Science and Technology, University of Crete, Herakleion, Greece

We investigate the nonlinear rheology of colloidal suspensions of varying interactions around their glass transition volume fraction. We focus primarily on the shear-melting behavior. We compare the response of hard spheres with that of model soft spheres (colloidal star polymers). We invoke the cage picture to identify the differences in the relaxation mechanisms in the two systems, with different effective volume fractions, based on rheological and DLS measurements. The shear melting of the different glasses is measured with large amplitude oscillatory and steady shear measurements. Remarkably, the yield values are comparable, a finding attributed to the particular structure of the stars. The rheological signatures of the yielded glasses exhibit similarities with other systems such as attractive glasses and flocculated suspensions. More importantly however, they exhibit some qualitative differences as well. We attempt at rationalizing these differences by drawing analogies to colloid polymer mixtures, as well as to fragile and ductile glasses.

Email: dvlasso@iesl.forth.gr

The Changing Face of Computational Rheology

Roger Tanner

Department of Aeronautics, University of Sydney, Australia

The Workshop has now been in operation since the first meeting in Providence, Rhode Island, in 1979. We are now in a full circle on Rhodos Island, and this talk will survey progress and changes that have occurred in nearly forty years of furious activity .The development of computer power has followed Moore's Law, and we can now begin to decide whether or not computational rheology has kept pace with this. New aspects of our subject continue to appear, and speculation about the future will close the presentation.

Email: rit@aeromech.usyd.edu.au

ORAL CONTRIBUTIONS

Rheology and Microscopic Rearrangements of Colloidal Glasses and Shear-Induced Crystals

N. Koumakis [1], G. Petekidis [1,2]

[1] Institute of Electronic Structure and Laser, Foundation for Research and Technology - Hellas (FORTH), Herakleion, Greece
[2] Department of Materials Science and Technology, University of Crete, Herakleion, Greece

We present linear and nonlinear rheology in suspensions of hard-sphere colloids with particular reference to the rheological behaviour of shear induced crystals. Using practically monodisperse hard spheres, we are able to examine glassy suspensions and give comparison to the rheology of their shear-crystallized counterparts. It is evident, that shear-induced crystallization causes a significant drop in the elastic modulus G' due to the structural rearrangements of crystal formation. The properties of rheological aging on glass and crystal are also probed. It seems that both glassy and crystal hard sphere solutions exhibit an increase of both G' and G" with the passage of time. Furthermore, the microscopic particle rearrangements during the shear-induced crystallization are followed by the technique of Light scattering Echo.

Email: nickk@iesl.forth.gr

Rheology of Attractive Hard Sphere Glasses and Gels

N. Koumakis [1], G. Petekidis [1,2], D. Vlassopoulos [1,2]
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We report the yielding behavior in colloids with hard sphere interaction plus a short-range attraction. The system is a suspension of nearly hard sphere colloidal particles and non-adsorbing linear polymer, which induces a depletion attraction between the particles. Hard sphere glass shows a simple yielding process at the strain corresponding to the maximum distortion of the cage; the structural arrest length scale. However attraction dominated glass show a two-step yielding process at different ranges of strain. We suggest the first step at low yield strain corresponds to the breaking of the attractive bonds between the particles and the second at larger strain to the cage breaking process. We also follow the transition from a low volume fraction gel with a single step yielding process to an attractive glass with a two-step yielding process.

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Ageing and Yielding in a Soft Colloidal Glass

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We have experimentally studied the aging and the yielding of a star > polymer with 128 arms with particular reference to behavior near the concentration of the glass transition. We investigated the strain response during and after a creep measurement. We applied stresses below and above the yield stress of the system and we found that there is an elastic recovery of strain, when the stress is removed. We noticed that below the yield stress there is a characteristic plateau of the strain, which shows that the material behaves as a solid, but when the applied stress is higher that the σ_y, the plateau disappears and the system flows as a liquid. Also we have found history dependent effects, which are interpreted in terms of aging and rejuvenation phenomena.

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Atomistic Monte Carlo Simulation of a Polymer Melt under a Flow Field by Employing Generalized Ensembles

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We present a new simulation methodology, which has a great potential for investigating the viscoelasticity of long-chain polymeric liquids of relevance even to systems and conditions used in practical polymer processing operations. The main idea of the new scheme is to combine two different thermodynamically-founded simulation algorithms: GENERIC (General Equation for the Nonequilibrium Reversible-Irreversible Coupling) Monte Carlo (MC) [1,2,3] and Non-Equilibrium Molecular Dynamics (NEMD) [4]. With the new methodology, we are able to relate properly chosen state variables representing nonequilibrium states of the system of interest in the frame of the GENERIC formalism to the corresponding real, physical variables that directly bring about the same nonequilibrium states. We achieve this by taking first advantage of GENERIC MC to drive quickly the simulated system to certain nonequilibrium (but steady-) states of interest, and by performing next NEMD simulations to obtain all the important dynamical information of the nonequilibrium states. As a simple test case, we have applied the new scheme to a relatively short chain, linear polyethylene melt, and results will be presented for its response to a shear flow field. More importantly, it is expected that our new methodology (when properly incorporated within a coarse-grained modeling scheme) would make it possible to efficiently study the true reptation regime of polymer melts.

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Steady Bubble Rise and Deformation in Bingham Fluids and Conditions for Their Entrapment

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We examine the buoyancy-driven rise of a bubble in a Bingham fluid assuming axial symmetry and steady flow. Bubble pressure and rise velocity are determined, respectively, by requiring that its volume and center of mass remain constant. The continuous constitutive model suggested by Papanastasiou is used to describe the viscoplastic behavior of the material. The flow equations are solved numerically using the mixed finite-element/Galerkin method. The nodal points of the computational mesh are determined solving a set of elliptic differential equations to follow the often large deformations of the bubble-surface. The accuracy of solutions is ascertained by mesh refinement and by predicting very accurately previous experimental and theoretical results for Newtonian fluids. We determine the bubble shape and velocity and the shape of the yield surfaces for a wide range of material properties. Besides the yield surface away from the bubble which surrounds it, unyielded material can arise either behind the bubble or around its equatorial plane in contact with the bubble. As the Bingham number increases, the yield surface at the equatorial plane and away from the bubble merge and the bubble gets entrapped. When the Bond number is small and the bubble cannot deform from spherical the critical Bingham number is 0.143, i.e. it coincides with the critical Bingham number for the entrapment of a solid sphere in a Bingham fluid. As the Bond number increases allowing the bubble to squeeze through the material easier, the critical Bingham number increases as well.

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Weakly Compressible Poiseuille Flows of a Bingham Fluid

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We solve the steady, creeping, weakly compressible plane and axisymmetric Poiseuille flows of a Herschel-Bulkley fluid. Under the assumption of weak compressibility, the pressure gradient is a function of the axial coordinate and satisfies a non-linear equation that involves the material parameters and the density of the fluid. The density is calculated by means of an equation of state. In the present work, both the linear and the exponential equations of state are considered. For a given pressure, the nonlinear equation can be solved using the Newton method and by means of numerical integration the pressure distribution can be calculated across the flow direction. The velocity profiles across the channel can then be constructed. It is shown that the position of the yield point approaches the wall as one moves upstream from the channel or capillary exit. As a result, for a given channel-length no flow can occur if the imposed pressure at the inlet is below a critical value.

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Numerical Simulation of Calendering of Viscoplastic Materials

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Numerical simulations have been undertaken for the process of calendering viscoplastic sheets with a finite thickness. The Finite Element Method (FEM) is used to provide numerical results for both cases of a fixed entry thickness or a fixed exit thickness under two-dimensional steady-state conditions. The Bingham-Papanastasiou model of viscoplasticity is used, which is valid for all ranges of deformation rates. Part of the solution is finding the separation point and the shape of the free surface of the exiting sheet. Yielded/unyielded regions are found *a posteriori* for a range of the dimensionless yield stress or Bingham number from the Newtonian limit (viscous fluid) to the fully plastic one (plastic solid). The 2-D FEM results show limited unyielded regions between the rolls, in disagreement with the Lubrication Approximation Theory (LAT), which predicts erroneous extended unyielded regions. However, LAT is very good at predicting the excess sheet thickness over the thickness at the nip, the pressure distribution and all engineering quantities of interest in calendering. Viscoplasticity leads to excess sheet thickness (at most 33% for extremely viscoplastic materials) as the dimensionless yield stress goes from zero (Newtonian behaviour) to one (plastic behaviour). All engineering quantities, given in a dimensionless form, increase substantially with the departure from the Newtonian values.

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Squeeze Flow of Carbopol Gels

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Carbopol gels are viscoplastic materials that do not seem to have any elasticity. The squeeze flow test is a convenient method of measuring their yield stress. As a force is applied to a plate to squeeze the material, at a certain moment the movement of the plate stops and the material cannot be squeezed anymore. This finite height can be related to the yield stress of the material.
Experiments and simulations have been conducted for this type of squeeze flow with a constant force. The finite height is measured for different configurations and squeeze forces. The numerical simulations reveal interesting yielded/unyielded regions as the phenomenon progresses in time. Finally, a simple formula proposed by Covey and Stanmore in 1981 and based on the lubrication approximation, is applied to find the yield stress from the limiting height, and appears to give acceptable results.

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Bifurcation Analysis of Flow Instabilities in Polymer Melts during Extrusion

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We use the concept of timesteppers [Kevrekidis et al., Comm. Math. Sciences, 1 (2003) 715] to perform systematic numerical bifurcation and stability analysis of a distributed-parameter model describing the dynamics of a plane Poiseuille flow of an Oldroyd-B fluid during extrusion with slip at the wall. In the past, it has been shown that due to the interplay between the nonmonotonicity of the slip equation and the viscoelasticity, the steady-state flow curve contains regimes with stable and unstable equilibria while self-sustained periodic oscillations appear when an unstable steady state is perturbed.
Here we further investigate the onset of such instabilities. We show for the first time that the loss of stability of steady-state solutions to sustained oscillating ones takes place through a subcritical Hopf bifurcation while the branch of stable periodic solutions loses stability through a critical point of limit cycles. This combination implicates the coexistence of stable steady states with stable and unstable periodic solutions in a narrow range of values of flow rates that can drive the system to abrupt loss of stability and under certain operating conditions to bursts.

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Cavity Filling Process Modeling by Rheological Characterization and Large Scale Computation

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Thermal cavity filling is at the heart of many polymer processes used to impart desirable surface structure on polymer items. Depending on the precise temperature-pressure history imposed, the produced item may not have the exact shape of the mold surface due to viscoelastic rebound in the pressure release stage. To minimize surface rebound, we developed a non-isothermal, viscoelastic free-surface flow model of the cavity filling process based on the DEVSSG-FEM. This novel model follows the polymer flow in the cavity through all process stages that traverse the polymer's glass transition. Although the model is two-dimensional, it applies a shape-dependent correction for three-dimensional flow effects on the polymer mass balance. Necessary parameters of the PTT rheological model employed are fitted from linear and nonlinear viscoelastic measurements and from direct process observables such as applied external force and total surface rebound. Due to the high computational requirements imposed by the multi-mode viscoelastic model and to the large number of cases that needed to be computed for parameter fitting, high-throuput computing on a network of distributed processors was employed. Results include thermal, stress and deformation field histories that showcase the model's predicting capability.

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On Kinetic Models for Dilute Suspensions of Rigid Rods

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We discuss the existence theory for certain kinetic models for the modeling of dilute suspensions of rigid rods. The model consists of a coupled Smoluchowski equation describing the evolution of a micro-scale together with Stokes flow for the motion of the solvent. For certain parameter values, the velocity gradient versus stress relation defined by the stationary and homogeneous flow is not rank-one monotone. We consider the evolution of possibly large perturbations of stationary flows and prove that, even in absence of a microscopic cut-off, discontinuities in the velocity gradient cannot occur in finite time.

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On the Gas Penetration in Periodically Constricted Circular Tubes Filled with Viscoelastic Liquids

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We examine numerically the displacement of viscoelastic liquids by pressurized air from harmonically undulated tubes of finite length. This unsteady process gives rise to a long open bubble of varying radius, increasing length and surrounded by the liquid. The viscoelastic part of the liquid stresses is subject to either the exponential PTT or the Oldroyd-B constitutive law. In general, the thickness of the liquid film that remains on the tube wall is non-uniform. Under creeping flow conditions, it varies periodically, but with a phase difference from the tube radius. The liquid fraction remaining in each periodic segment of the tube increases as the ratio between the minimum and maximum of the tube radius, decreases, whereas it tends to an asymptotic value for straight tubes, as the wavelength of the tube undulation increases, although here the flow is accelerating. The liquid fraction also depends strongly on the solvent viscosity and the exponential parameter of the PTT model. It increases as any of the two parameters decreases and tends to the Newtonian limit as takes large enough values. At high values of the Reynolds number, the film thickness increases with the axial distance, and the periodicity of the velocity and stress fields ahead of the bubble tip, which exists under creeping flow conditions, is broken. At even higher Reynolds numbers, recirculating vortices develop inside each tube expansion and when also decreases significantly, nearly isolated bubbles are formed in each tube segment, while the free surface exhibits corrugations.

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Viscoelastic Analysis of Complex Flows: From the Constitutive Model through the Numerical Simulations and their Experimental Validation

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In this work we present some interesting results (i.e., helical flow and big vortices) concerning the viscoelastic behavior of branched polymer melts in 3D complex flow conditions. Most of the studied 3D geometries are natural generalizations of the 2D classical benchmark flow problems, like the planar contraction flow or the pressure-driven cavity flow. The Single-equation version of the eXtended Pom-Pom (S-XPP) model is implemented to describe correctly the complex rheology of branched polymers. The numerical results are compared with the experimental data in terms of flow kinematics and stress distribution characterized by flow-induced birefringence.
The main conclusion concerning the constitutive model is that although mathematically equivalent, not all the versions could be implemented efficiently in numerical flow analysis, especially in the presence of geometrical singularities. Our study clearly shows that a full 3D analysis in combination with an efficient constitutive model are definitely required for describing correctly the flow behavior under different experimental flow conditions.

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Dynamic K-L Analysis of Coherent Structures Based on DNS of Turbulent Newtonian and Viscoelastic Flows

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The turbulent dynamics corresponding to Direct Numerical Simulation (DNS) data of Newtonian and viscoelastic turbulent channel flows is analyzed here through a projection of the velocity fields into a set of Karhunen-Loeve (K-L) modes, large enough to contain, on the average, more than 90% of the fluctuating turbulence energy.

Previous static K-L analyses have demonstrated a dramatic decrease in the K-L dimensionality (and, correspondingly, the number of modes carrying most of the turbulent energy) accompanying the presence of viscoelasticity in turbulent channel flows; this is consistent to the increasing importance of large coherent structures for viscoelastic turbulent flows, as also has been revealed in flow visualizations of DNS data. We exploit this feature here in using the K-L modes dynamically to gain quantitative insights into the behavior of the overall flow dynamics, which may eventually help to explore approaches towards a low-dimensional modeling of the viscoelastic turbulence.

A representational entropy constructed from the projection coefficients is used in conjugation to the calculation of the fluctuating kinetic energy to provide additional evidence that viscoelastic turbulent flow is better organized than in the Newtonian limit. Moreover, dynamic correlation analysis between pairs of K-L coefficients showed a systematic increase in the time scales characterizing dynamic turbulent events with viscoelasticity. These correlations have distinct pulse behavior characteristic of intermittence and quasi-periodicity in turbulence.

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A log-Exponential Mapping for the Preservation of Positive Definiteness in the Numerical Integration of Viscoelastic Constitutive Models

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We present a new method in order to integrate the evolution equation for a symmetric and positive definiteness second order tensor (SPD) which results when modeling the transient flow behavior of viscoelastic fluids. The method is based on the log-conformation representation, also reported earlier by Fattal & Kuprferman, JNNFM 2004 & 2005, the application of the Cayley-Hamilton theorem for second order tensors and an additional mapping which ensures that the tensor remains always bounded. The algorithm is used for the simulations of viscoelastic turbulent channel flow, which have been received great attention since mid 90's with ultimate goal to enlighten the phenomenon of maximum drag reduction usually observed in wall bounded flows. The main new feature for the implementation of the proposed scheme is relied on a second order finite difference multigrid diffusion which guarantees the positive definiteness of the conformation tensor. Sample results will demonstrate the window of parameters where the new algorithm can prove to be of uselfulness to numerical simulations of viscoelastic turbulent flow.

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POSTER CONTRIBUTIONS

A Generalized Single-Conformation Tensor Viscoelastic Model Based on Principles of Non-Equilibrium Thermodynamics

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Guided by the GENERIC and bracket formalisms of non-equilibrium thermodynamics [1,2], we present a generalized single-conformation tensor based viscoelastic model which reduces to known rheological models, such as the Giesekus, the Phan-Thien/Tanner and the FENE-P ones, under certain limiting conditions. The new model incorporates the dissipation or friction matrix corresponding to the Giesekus model but, in addition, accounts for finite-extensibility effects as well as for anisotropic effects in the relaxation spectrum in the spirit of the White-Metzner model. Key in the new model are two functions: the free energy function (associated with the elasticity of the fluid) and the friction matrix (associated with dissipation effects). In essence, the new model extends or corrects the Giesekus model to account for the finite extensibility of the chain at high deformation levels. We will present the predictions of the model in the simple shear and 1D-extensional flows, we will discuss its capability to fit available rheological data for a number of polymers, and we will comment on the opportunity it offers to accommodate within the constitutive equation more complicated, bounded expressions for the free energy of the deformed liquid such as those proposed for highly elastic materials.

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Numerical Simulations of Flow in a Variable-Speed Corotating Twin Screw Extruder

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The flow field and mixing pattern in a variable speed corotating intermeshing twin-screw extruder is studied. In this extruder, the two screws have different number of flights and rotate at different speeds. Results from numerical simulations and flow visualization experiments suggest that this extruder exhibits superior distributive mixing in comparison with a regular corotatingg twin-screw in which the screws are identical and rotate at the same speed. In addition, this new screw design exhibits a more positive flow displacement action and a shorter average residence time.

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Rheological Characterization of Foodstuff Used in Rolling Experiments and Modeling via Integral Constitutive Equations

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The calendering and rolling processes are used in a wide variety of industries for the production of rolled sheets or films of specific thickness and final appearance. The acquired final sheet thickness depends mainly on the rheological properties of the material. Materials which have been used in the present study are foodstuff (such as mozzarella cheese and flour-water dough) used in food processing. These materials are rheologically viscoplastic-elastic. They have been rheologically characterized using a parallel-plate, an extensional, and a capillary rheometer at room temperature. Based on the linear and non-linear viscoelastic and viscoplastic data, two constitutive equations have been formulated, namely a viscoplastic Herschel-Bulkley model and a visco-elasto-plastic K-BKZ model with a yield stress. For cases where time effects are unimportant, the viscoplastic Herschel-Bulkley model can be used. For cases where transient effects are important, it is more appropriate to use the K-BKZ model with the addition of a yield stress. Finally, the wall slip behaviour of dough was studied in capillary flow, and an appropriate slip law was formulated. These models adequately characterize the rheological behaviour of bread dough and constitute the basic ingredients for flow simulation of dough processing, such as extrusion, calendering and rolling.

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Predicting the Behaviour of Nylon-6 through Industrial Spin Packs

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In fiber spinning of polyamide-6 (nylon), the spin pack is equipped with a range of wire-mesh filters through which the melt must pass to become fine fibers. The problem of the prediction of the fluid dynamics pattern through wire-mesh filters is akin to flow through porous media, where Darcy's law may be used to predict the pressure drop vs. flow rate of the system. Experiments of a Newtonian silicone oil and polyamide-6 have been run in a pilot-plant equipment, and the pressure results are given for different wire-mesh filters. Then, fitting of the data with Darcy's law is carried out with the aim of finding the ratio K/H, where K is the permeability of the porous media and H is the height of the porous media. These values are then used for testing all experimental pressure drop data against the model predictions. Finally, pilot-plant results are given for spin-packs containing spinnerets, filters, and metal sand.

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Numerical Simulation of the Extrusion of Strongly Compressible Liquid Foams

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The axisymmetric and plane extrusion flows of a liquid foam are simulated assuming that the foam is a homogeneous compressible Newtonian fluid that slips along the walls. Compressibility effects are investigated using both a linear and an exponential equation of state. The numerical results confirm previous reports that the swelling of the extrudate decreases initially as the compressibility of the fluid is increased and then increases considerably. The latter increase is sharper in the case of the exponential equation of state. In the case of non-zero inertia, high compressibility was found to lead to a contraction of the extrudate after the initial expansion, similar to that observed experimentally with liquid foams, and to decaying oscillations of the extrudate surface. The time-dependent calculations show that the oscillatory steady-state solutions are stable. These steady-state oscillatory solutions are not affected by the length of the extrudate region nor by the boundary condition along the wall.

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Annular Poiseuille Flow of a Newtonian Liquid with Non-monotonic Slip along the Walls

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The Poiseuille flow of a compressible Newtonian fluid assuming that slip occurs along the wall is studied. Different slip models relating the wall shear stress to the slip velocity are employed. In the case of linear slip, it is easily shown that the slip velocity along the inner cylinder is always greater than the slip velocity along the outer cylinder. In the case of a non-monotonic slip equation, there exist linearly unstable steady-state solutions corresponding to the negative-slope regime of the slip equation. As a result, the resulting flow curve is also non-monotonic with an intermediate unstable negative-slope branch, which corresponds to the stick-slip extrusion instability regime. It is shown for small radii ratios $\kappa=R_1/R_2$, two stable steady-state solutions are possible in a certain range of the volumetric flow rate. As a consequence, the stick-slip instability regime is reduced in size and eventually disappears as κ is decreased. This provides an explanation for the fact that the stick-slip instability is not observed in annular extrusion experiments.

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The Temperature Dependence of the Rouse Mode Relaxation Spectrum and Zero Shear Rate Viscosity in Cis-1,4-Polybutadiene: Results from Long Atomistic Molecular Dynamics Simulations down to the Glass Transition Temperature T_g

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A well-relaxed atomistic configuration of a 32-chain C_{128} cis-1,4-polybutadiene (*cis*-1,4-PB) system has been subjected to long (on the order of a few microseconds) molecular dynamics (MD) simulations in the NPT ensemble using the united-atom forcefield introduced by Smith and Paul [1] on the basis of quantum chemistry calculations. This allowed us to study in detail the temperature dependence of the Rouse-mode relaxation spectrum of *cis*-1,4-PB over a wide range of temperature (from T=430K down to 165K) and pressures (from P=1 atm up to P=3.5 kbar) conditions. Results are presented here for: (a) the time decay of the autocorrelation function of the normal coordinates (Rouse modes), (b) the single chain intermediate coherent dynamic structure factor, $S_{\mathrm{coh}}(q,t)$, and (c) the intermediate incoherent dynamic structure factor, $S_{\mathrm{inc}}(q,t)$, for different values of the wavevector q. By mapping our MD simulation results onto the Rouse model, we have also been able [2] to extract a prediction for the zero shear rate viscosity of the simulated cis-1,4-PB system as a function of temperature (for temperatures as low as down to T_g) and compute its fragility index.

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