Nonequilibrium Thermodynamics and Complex Fluids IWNET 2006

Rhodes, Greece
September 2 – 7, 2006

Chair	Session
H.C. Öttinger	Non-equilibrium thermodynamics and statistical mechanics
T. Tzavaras	Multiscale modeling and molecular simulation
M. Kröger	Non-equilibrium thermodynamics and molecular dynamics
M. Grmela	Complex fluid deformation and rheology: Theories and thermodynamic relationships
A.N. Beris	Non-equilibrium thermodynamics: Approaches and formalisms
B.J. Edwards	Coarse-graining and mesoscopic dynamics – some mathematical aspects
V.G. Mavrantzas	Applications to complex materials: glasses, micelles, colloids, blends, interface

Figure 1:
Port of Rhodes.

The application of thermodynamics to the rheology of complex fluids is by no means obvious. The international workshop IWNET 2006, jointly organized by FORTH-ICE/HT, the university of Patras and the Hellenic Society of Rheology highlighted the most recent advances in the related fields, in particular, new theoretical developments and state-of-the-art modeling/simulation techniques. The workshop took place in the vicinity of the medieval city of Rhodes, Greece from 2-7 September 2006.

The workshop started on Sunday afternoon in a convention center close to the beach, with some welcome remarks by V.G. Mavrantzas. Session 1 was headed off by D.J. Evans with a review about the fluctuation and non-equilibrium free energy theorems – Theory and Experiments. Next, K. Valanis discussed about non-affine deformation and the basis of material irreversibility. The session was completed by J.-P. Eckmann who reviewed recent progress in our understanding of non-equilibrium steady states.. Session 2 focussed on i) the construction of entanglement networks, their characterization, and their usage for the development of slip-link models and ii) the efficient generation of equilibrated polymer samples for atomistic simulation. C. Tzoumanekas and M. Kröger presented their geometric approaches [1 - 3] to efficiently calculate entanglement networks and offered some applications on the testing of molecular theories. K. Kamio successfully compared classical annealing methods with the modern geometric algorithms. V. Harmandaris, and also C. Tzoumanekas offered a route to perform the challenging back-mapping from coarse-grained to atomistic configurations. Applications for these methods have been discussed, such as the localization and the characterization of entanglements and their dynamical properties. Session 3 offered a collection of talks where stress-optical behavior (C. Baig), microscopic chaos (B. Todd) in both shear and elongational flows [4], as well as shear bandings (W. Briels), and Hamiltonian based algorithms (B.J. Edwards) received some attention. Session 4 was kicked off by A. Onuki with an excellent plenary talk. He presented a simple van der Waals extension [5] of hydrodynamic equations to model bubble formation in the presence of temperature gradients. P.J. Daivis presented a phenomenological, thermodynamical framework to split the work done in taking a viscoelastic fluid from equilibrium into a shearing steady state into elastic (reversible) and viscous (irreversible) parts. M.T. Downton reported about dynamical heterogeneities in cooled binary mixtures to understand the low temperature breakdown of the linear relationship between viscosity and translational diffusion. B.U. Felderhof talked about the damping of capillary-gravity and Marangoni water waves upon adding a small amount of oil, an effect used already in ancient times by sailors to flatten the water surface. H.R. Brand expanded general macroscopic equations to arrive at a minimal model which accounts for many experimental observations, and expressed viscosities in terms of essentially five material dependent parameters. A. Minami developed a nonlinear elastic theory (phase fluid model) to study dislocation formation in binary alloys. For this model the free energy is expressed in terms of composition and displacement vector and takes into account crystal symmetry. Dislocations are spontaneously formed at interfaces on quench [6]. B.J. Edwards talked about thermodynamics of non-isothermal flows and the concept of

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entropic elasticity. Particularly, he investigated the validity of the temperature equation used in several commercially available flow solvers. In the following discussion D. Evans mentioned that the absence of 0th law of thermodynamics for complex fluids is the main origin of difficulty to uniquely define temperature characterizing nonequilibrium steady states. After lunch, E. van Ruymbeke reported about a general methodology to predict the linear rheology of branched polymers employing branch friction, while predicitions strongly depend on the definition of a branch contour variable. H. Pleiner combined the nonlinear hydrodynamic description of viscoelastic fluids with a general 2-fluid hydrodynamic description.to arrive at a hydrodynamic model for disperse polymers and colloids. He mentioned a number of related, yet unsolved problems. A. Menzel presented selected nonlinear physical properties of liquid crystalline elastomers, where network deformation is coupled to the elastic energy of the director field. C. Löschke talked about dilute suspensions of rodlike molecules and the Doi model as a multi-scale model and discussed stability issues. Session 4 was followed by a poster and coffee session, before participants left for an excursion to Lindos acropolis. Session 5 opened with a plenary talk by G. Nicolis about an extended thermodynamic approach for non-equilibrium systems restoring, at least in part, the universality of the traditional thermodynamic description. He presented a multi-level approach involving master equations (probabilistic approach), generalized entropies and kinetic potentials towards the stochastization (Markov partition) of dynamics in phase space. The breakdown of variational structure and analyticity in the presence of several attractors.and higher order bifurcations limits the possibility to come up with a classification of nonequilibrium dynamical scenarios in the near future. Next, H.C. Öttinger presented beyond-equilibrium thermodynamics of boundary conditions embedded in the GENERIC framework [7, 8] and presented two examples: the diffusion cell and wall slip to illustrate the concept of dynamical boundary conditions.

D. Jou presented extended thermodynamics of polymers and superfluids and gave some arguments on why to use the viscous pressure tensor as the relevant variable [9]. M. Grmela focused on relating the GENERIC approach [7] to the viewpoints presented by G. Nicolis with whom he basically agreed. He offered new routes to understand the difference between turbulent kinematics in simple and polymeric fluids. In his talk M. Hütter presented momentum density, energy, and deformation gradient as relevant variables to embed the theory of elasto-viscoplastic deformations into the GENERIC formalism. He splits volumetric and deformation effects, puts forward arguments to use the so called current state rather than reference state description and proposes expressions for the driving forces for irreversible processes including a mass diffusion term which were hereafter discussed in more detail by D. Bedeaux. He further talked about the possible difference between barycentric and translational velocity and the corresponding implications. So far, there is no clear experimental evidence or disagreement with these predictions, originally proposed by H. Brenner, but D. Bedeaux proposed some experimental setups to test these puzzling ideas which would imply a (small) correction of the Navier-Stokes equations. Finally, F. Vasquez connected non-equilibrium fluctuations with path integrals. Session 6 focused on mathematical

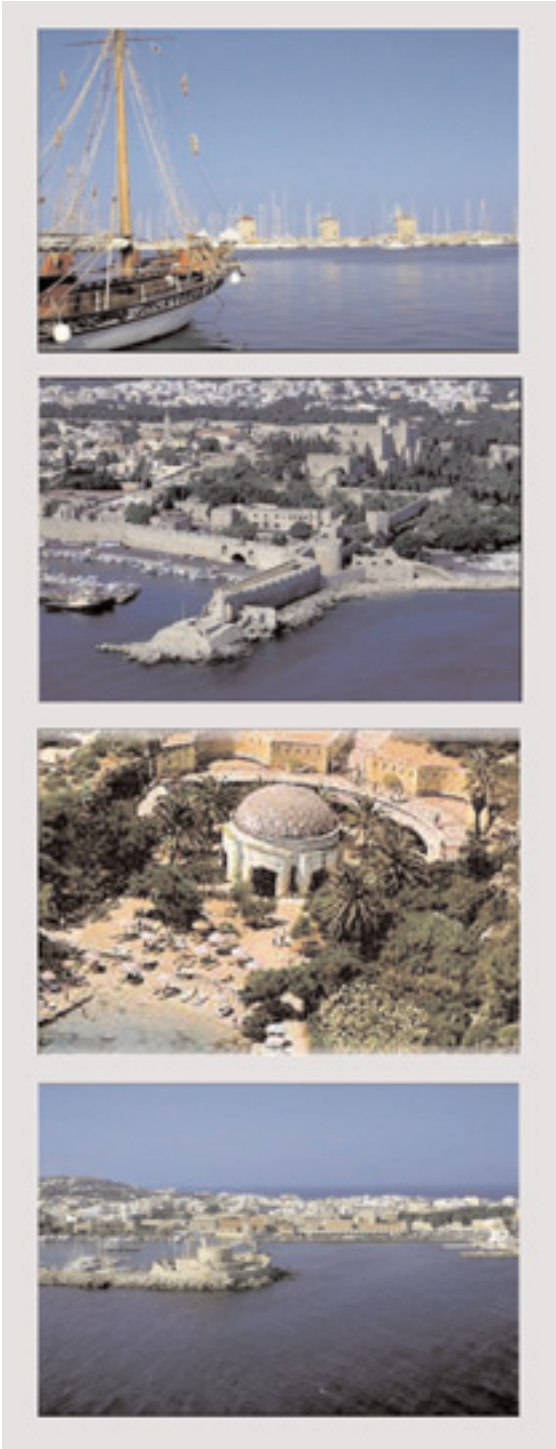

Figure 2:
Impressions from the Island of Rhodes, Greece.

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aspects of coarse-graining which were then summarized by M.A. Katsoulakis and P. Plechac in their lectures. Talks on the last workshop day, collected in Session 7, offered a range of applications for the ideas presented earlier in the workshop. The session started with a plenary lecture held by C.A. Angell about ergodicity-breaking in glass-forming liquids, and relaxation processes in glassy states.

The organizers succeeded in generating a very pleasant, personal and hence stimulating atmosphere. In summary, a number of issues came up that need the attention of this community in the next years, as suggested by H.C. Öttinger: (1) Nonisothermal experimental rheology (energy/entropy balance should be considered in addition to the momentum balance), (2) Boundary thermodynamics [8], (3) Toy models and rigorous results to clarify fundamental concepts and to guide and strengthen empirical frameworks, (4) Multiscale modelling with a systematic nonequilibrium methodology (superatoms, T-dependence of renormalized potentials, rescaling of time to account for renormalized friction or dissipation?) and also locally adaptive and equation-free methods., (5) The theory of fluctuations and related conclusive simulations, (6) Numerical integration schemes with thermodynamic structure, (7) Total number of entanglements as dynamical variable for polymer melts, (8) Substances and phenomena: Turbulence, Glasses, Granular media, Suspensions, Colloids, Polymer melts for all kinds of chemical structure. There are also topics which are still on the table but should be resolved within the next few years via (a) A conclusive review on the proper implementation and usage of NEMD, SLLOD, DOLLS, and related algorithms, (b) Clear recipes on how to use energy and entropy balances rather than introducing the notion of nonequilibrium temperature, (c) A final opinion about Brenner's hydrodynamics with diffusion.

The 5th IWNET 2009 will be organized by M. López de Haro and F. Vázquez to take place in Cuernavaca, Mexico.

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Figure 3 (left):
Vlasis Mavrantzas, local organizer, surrounded by participants.
(photo taken by Brian Edwards)

Figure 4:
Part of Rhodes firtification of the 14th–15th century built by the Knights of Saint John.
(photo taken by Brian Edwards)

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