

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ & ΕΡΕΥΝΗΤΙΚΟΥ ΙΝΣΤΙΤΟΥΤΟΥ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ ΚΑΙ ΧΗΜΙΚΩΝ ΔΙΕΡΓΑΣΙΩΝ ΥΨΗΛΗΣ ΘΕΡΜΟΚΡΑΣΙΑΣ

ΟΜΙΑΗΤΗΣ : Eduard Oleinik, Professor of Polymer Science, Institute of Chemical Physics, Russian Academy of Sciences, Moscow, Russia

ΘΕΜΑ : New Approach to Plastic Deformation of Glassy Polymers

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων, ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Πέμπτη, 24 Νοεμβρίου 1994

ΩΡΑ : 5.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Extensive measurements of stored energy of cold work (Deformation Calorimetry Technique), recovery of residual strain and release of the stored energy upon heating (Def. Calorim., DSC, TMS) were performed with: linear and cross-linked glassy polymers, several semi-crystalline polymers containing a glassy amorphous phase and immiscible blends based on PC. The results of these experiments we could not explain and understand in the framework of current models of polymer deformation and the necessity for a new model for glassy polymer inelastic deformation has appeared. A main feature of the process is the storage by a sample during its cold work of a high amount of internal energy, which starts at the very beginning of straining. The level of stored energy reaches 70-95% of the mechanical work expended in deformation at low strains (below ϵ_y) and 30-45% at higher strains. The stored energy shows the tendency to level off at compressive strains 25-35% (room temperature) in most cases. The fraction of the expended work stored in polymeric glasses is much higher compared to metals, where it is normally less than 5-10% and seldom as high as 15%. We were able to show that the energy storage in polymer glasses appears due to stress-biased formation of special shear "defects"-Plastic Shear Transformations (PST)-small, local-scale structural rearrangements. Each PST is carrying small strain (shear displacement) and is surrounded by an elastic field. All these fields are the microscopic carriers for the sample macroscopic stored energy of cold work. Nucleation of PSTs is not connected with the free volume changes in a sample and with the conformational rearrangements in macromolecules. The collection of PSTs brings the glass into a new excited metastable thermodynamic state and all following processes happening in polymer upon loading such as yielding, steady plastic flow, deformation hardening and softening, formation of cracks, crazes or shear bands, are going in the new but not native state of the glass. Macroscopic yielding happens only when the PST concentration reaches some critical level, characteristic for given polymer and strain conditions. The second important stage of the deformation process is the PST's termination (death). The termination is the process responsible for dissipation of the stored upon loading energy excess. If the dissipation is not going effectively, the energy excess may dissipate through nucleation and development of cracks or crazes and the material may show brittle behavior. A necessary part of the PST termination process is the conformational rearrangements in macrochains. Because the major part of macrostrain is collected in the PST's nucleation but not in termination, the whole inelastic deformation of glassy polymers is close to pure anelasticity. The comparison of deformation behavior of crystals and glasses is considered in the presentation also.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

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ΟΜΙΛΗΤΗΣ : Prof. Peter Hall, Department of Pure and Applied Chemistry,
University of Strathclde

ΘΕΜΑ : Contrast Matching Small Angle Neutron Scattering Techniques to
Monitor Pore Development in Activated Carbons

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 26 - 9 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Activated carbons are important as industrial adsorbents and as catalyst supports to make more specifically acting carbons attempts are being made to produce materials with well defined pore sizes. A precise understanding of how pores develop in carbons following gasification is important. Small angle neutron scattering has been applied to this problem. Scattering from dry samples is shown to result from scattering by open porosity, closed porosity and interparticle effects. Contrast matching with deuterated toluene eliminates scattering from open pores and interparticle effects thus enabling the influence of closed porosity to be investigated. Pore development in two carbons, phenolic resin char (prc) and Pittsburgh #8 coal char are compared. It is shown that pore development in prc takes place by opening closed porosity whereas pore developments in Pittsburgh #8 char is by the creation of new pores.

ΣΕΜΙΝΑΡΙΟ

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ΟΜΙΛΗΤΗΣ :PROF. RICHARD M. LAMBERT,
Cambridge University, UK

ΘΕΜΑ :What can model catalysts teach us about real
systems?: Two case studies

ΤΟΠΟΣ :Αίθουσα σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ :Δευτέρα, 19-9-1994

ΩΡΑ :12:00

ΠΕΡΙΛΗΨΗ:

Experiments on well defined single crystal surfaces can significantly increase our understanding the behaviour of real catalysts. This is illustrated by two examples:

- * *CO oxidation over Pt/CeO₂ where the properties of the metal/metal oxide interface are critically important*
- * *Acetylene coupling over Pd/Au where activity and selectivity are strongly dependent on particle size and surface composition.*

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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ΟΜΙΛΗΤΗΣ : Prof. Wolfgang Göpel, Institute of Physical and Theoretical Chemistry and Center of Interface Analysis and Sensors, University of Tübingen

ΘΕΜΑ : Charge Transfer Reactions at oxide Interfaces: Combined Spectroscopic and Transport Studies

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τετάρτη, 27 - 7 - 1994

ΩΡΑ : 12.00

ΠΕΡΙΛΗΨΗ : After a short discussion of model systems, experimental details are presented on systematic studies of phenomenological properties and microscopy and spectroscopy at oxide-based sensors and catalysts. Four different case studies are then described for chemical sensing and heterogeneous catalysts with "prototype materials":

- . surfaces of ideal single crystals ($\text{ZnO}(1010)$).
- . electron conduction materials (SnO_2)
- . mixed conduction (Pt/TiO_2) and
- .. ion conduction materials (Pt/ZrO_2).

Particular emphasis will be put on the atomistic understanding and a correlation between chemical sensor and catalytic properties.

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ΟΜΙΛΗΤΗΣ : Professor Christos Takoudis, Chemical Engineering
Department, Purdue University, West Lafayette, Indiana,
USA

ΘΕΜΑ : Relationships Between Microelectronic Material Properties
and Processing Environments

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Πέμπτη, 30 - 6 - 94

ΩΡΑ 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Chemical cleaning and etching of semiconductor surfaces as well as growth of thin films on substrate surfaces are studied with several spectroscopies and microscopies.

Surface infrared spectroscopy, X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy are used to study Si(100) and Si(111) surfaces in chemical cleaning processes. The morphology of the substrate surfaces is examined with scanning tunneling microscopy, atomic force microscopy, and optical microscopy. Novel two-step etching techniques involving a treatment with dilute HF followed by a pH-enhanced dilute - HF solution are shown to result in impurity-free and atomically smooth surfaces.

In situ emission Fourier Transform Infrared (FTIR) spectroscopy is used in the chemical vapor deposition of silicon, thermal oxide thin film growth, and wafer cleaning. Complementary information is obtained with ex situ analyses of semiconductor surfaces with XPS, ellipsometry and microscopies. These experimental studies coupled with theoretical models, are discussed in the context of interrelationships between processing environments and microelectronic material properties.

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ΟΜΙΛΗΤΗΣ : Professeur. A. Frennet, Catalyse Heterogène, Université libre de Bruxelles

ΘΕΜΑ : Transient Kinetics in Catalysis by Metals

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Πέμπτη, 23 Ιουνίου 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : The various kinetic methods and concepts that were successively developed since Langmuir are summarized. Transient kinetics concerning some systems, namely CO-H₂, conducted on metal catalysts are very briefly reviewed.

The conditions of applicability of the transient method are analyzed in terms of TOF and coverage in active intermediates. Some results concerning informations on the alloying effect of Rh with Ib metals (Cu, Ag) provided by the transient method applied to the kinetic studies of the CH₄-D₂ exchange reactions are presented. In the case of ethane hydrogenolysis, one of the most studied reactions as model for highly demanding reactions, it is analyzed how the independent use of each of the kinetic methods may be misleading in the analysis of the reaction mechanism. On the contrary, the combined information provided by steady state kinetic studies and transient kinetic studies, both conducted with labelled molecules, makes it possible, in this particular case, not only to determine the reaction scheme, but to derive the rate, back and forth, of the successive elementary steps of that reaction. It is concluded that studies under such conditions, the ethane hydrogenolysis reaction can be considered as a chemical probe of the catalytic properties of metal surfaces in their catalytically working conditions.

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ΟΜΙΛΗΤΗΣ : Professor Reinhold Haberlandt, Universität Leipzig, Fakultät für Physik und Geowissenschaften

ΘΕΜΑ : Molecular dynamics simulations of diffusion in zeolites under different conditions

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τετάρτη, 22 Ιουνίου 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Molecular Dynamics (MD) calculations are of great importance to understand diffusion behaviour in zeolites. Here the diffusion of methane in zeolites of structure type LTA and the influence of exchangeable cations will be discussed. Small variations of the Lennard-Jones parameters (determining the window size) and the nature of the considered exchangeable cations are found to be of decisive importance for the observed dependences, leading to self-diffusivities which may both increase and decrease with increasing concentration. Taking into account the gradient of the chemical potential as a driving force for the diffusion process, the transport-diffusivity is found to increase with increasing concentration. The theoretical results are in satisfactory agreement with the experimental ones.

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ΟΜΙΛΗΤΗΣ : Professor Costas Pozrikidis, University of California, San Diego

ΘΕΜΑ : Παραμόρφωση ερυθρών αιμοσφαιρίων σε διατμητική ροή.

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Πέμπτη, 16 - 6 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Τα ερυθρά αιμοσφαίρια είναι μικρές υγρές κάψουλες που περιέχουν ένα υδατικό διάλυμα αιμογλοβίνης και περιορίζονται από μια βιολογική μεμβράνη με μοναδικές μηχανικές ιδιότητες. Η μεμβράνη παραμορφώνεται εύκολα σε διατμητική τάση αλλά διατηρεί τοπικά και ολικά την αρχική της επιφάνεια. Στην έρευνα αυτή, υπολογίζουμε την παραμόρφωση των αιμοσφαιρίων σε απλή διατμητική ροή βασιζόμενοι σε μια αριθμητική μέθοδο του οριακού ολοκληρώματος για διεπιφανειακή ροή. Οι υπολογισμοί δείχνουν την ανάπτυξη τάσεων στη μεμβράνη και θέτουν όρια στο μέγιστο ρυθμό διάτμησης πάνω από τον οποίο τα αιμοσφαίρια θα καταστραφούν.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

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ΟΜΙΛΗΤΗΣ : Prof. Y.C. Yortsos, University of Southern California

ΘΕΜΑ : Bubble Growth in Porous Media

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 14 - 6 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : We study bubble growth in porous media by visualization experiments, pore network simulations and statistical models. Problems relevant to solute diffusion by pressure decline ("Solution gas-drive") or heat transfer ("boiling") are discussed.

The growth of a single bubble is shown to be described by invasion percolation at small sizes and by Diffusion-Limited-Aggregation at large sizes. The delineation of these boundaries is derived. The rate of growth in porous media is different than in the bulk and obeys the scaling $E_g \sim t^{1/(D_f-1)}$, where D_f is the fractal dimension, compared to the classical $R_g \sim t^{1/2}$. It is also shown that the viscosity ratio plays a stabilizing role opposite to the classical viscous fingering problem, and enhances a Mullins-Sekerka type of instability. This effect is common to all phase-change processes in porous media.

The growth of multiple bubbles is analyzed in terms of the nucleation characteristics of the system. Competition between growing bubbles is controlled by mass (heat) transfer, where the classical Ostwald ripening is not relevant, contrary to the bulk. The growth regimes are characterised in terms of simple statistical models in many cases. Finally, concepts such as "the critical gas saturation", which denotes the onset of bulk gas flow are studied and related to the nucleation characteristics of the process.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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ΟΜΙΛΗΤΗΣ : Professor John P. O' Connell, Department of Chemical
Engineering, University of Virginia

ΘΕΜΑ : Computer Simulation of Model Surfactant Systems

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 14 - 6 - 1994

ΩΡΑ : 11.00 π.μ.

ΠΕΡΙΛΗΨΗ : Molecular dynamics simulations have been performed on individual and micellar surfactants to elucidate their structure and dynamics, which cannot be unambiguously determined from experiment. It is found that chain conformations and their variations with time are the most important factors controlling the behavior of such substances, especially in aggregates. Further, aggregates of chains, of surfactants and of surfactants with chain-like solutes are seen to have quite similar structure and dynamics.

The talk will discuss issues associated with micelles and with computer simulation. describe the potential energy models used for the molecular dynamics, and the principal results, including a video.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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ΟΜΙΛΗΤΗΣ : Professor Antony N. Beris, Department of Chemical Engineering, University of Delaware

ΘΕΜΑ : Pattern formation and bifurcations in the viscoelastic Taylor-Couette flow.

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 13 - 6 - 94

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Viscoelastic flow instabilities represent the limiting factor for enhanced production in many polymer processes, such as extrusion, blow molding etc. In other instances, as, for example, in viscoelastic flow past objects or viscoelastic flow through porous media, instabilities of the primary flow are associated with the onset of secondary flows which are suspected to be responsible for the observed increases in the flow resistance. This talk will present the analysis of the viscoelastic instabilities in a simple flow geometry, that represented by two independently rotating concentric cylinders, the Taylor-Couette flow.

Our work led to the elucidation of the bifurcation diagram of the viscoelastic Taylor-Couette flow problem near the onset of instability, for both axisymmetric and non-axisymmetric disturbances for an upper-convected Maxwell and an Oldroyd-B fluid models. This was achieved through a computer-aided linear and non-linear stability analysis based on efficient pseudospectral approximations. Most importantly, the recently developed theory of Hopf-bifurcations in the presence of symmetries was used in order to decide on the form and the stability of the flow patterns emerging after the primary (Couette) flow becomes unstable.

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ΟΜΙΛΗΤΗΣ : Dr. D.A. Sarigiannis, Commission of the European Union
Joint Research Centre, Institute for Systems Engineering and
Informatics, Industry and Environment Unit, Italy

ΘΕΜΑ : On the incorporation of safety and environmental concerns
in process systems synthesis

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τετάρτη, 8 - 6 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Currently, a variety of advanced mathematical programming or heuristic techniques are available to process engineers for process synthesis and optimization. Usually, however, safety or environmental considerations are not included in the optimization functions used for process synthesis. The question of the performance of process plants with regard to safety and environmental impacts is handled usually after plant design, synthesis and optimization has been completed. If enough operational data are available a full-scale quantitative risk assessment (QRA) is feasible. This is the current state of the art in process safety analysis.

This situation is, however, constantly challenged by increasingly stricter environmental regulations and ever increasing public concern for the safety and health impacts of industrial processes. In this lecture, an integrated methodology to incorporate safety and environmental concerns in the design and synthesis of novel process plants is presented., The array of mathematical techniques available for risk quantification are described, and the problems associated with reliable risk assessment in preliminary stages of design are discussed.

The second part of this talk presents a new approach to the synthesis of novel chemical processes and plants, one that takes effectively into account safety and reliability issues. Some examples of the application of this methodology to specific chemical and physical process (e.g. multicomponent separation) synthesis are also given.

The goal of this work is to provide the process engineering community with a new conceptual tool that would permit the economically efficient incorporation of safety and environmental concerns in the chemical industries of tomorrow.

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ΟΜΙΛΗΤΗΣ : Henri Benoît
Professeur Université de Strasbourg
Ancien Directeur Institut Chales Sadron, C.R.M.

ΘΕΜΑ : Neutron Scattering and Polymers

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 7 Ιουνίου 1994

ΩΡΑ : 7.00 μ.μ.

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ΟΜΙΛΗΤΗΣ : Dr. Vlas Mavrantzas, University of Delaware Department
of Chemical Engineering

ΘΕΜΑ : Surface Effects on the Structure and Rheology of Polymer
Solutions

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 17 - 5 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : A thermodynamic approach is followed for the study of the structure and rheology of polymer solutions above a solid surface, neutral or adsorbing. The analysis starts with the derivation of a set of evolution equations describing the conservation of mass and momentum in a viscoelastic medium as well as the evolution of its structure at the macroscopic level. The possibility for a stress-induced polymer migration mechanism is also included in the derivation. The most important quantity entering the evolution equations is the total energy (Hamiltonian H) of the system. To calculate H , we resort to a microscopic model for the description of polymer conformations near the surface as imposed by the applied flow field. This is accomplished through the use of a diffusion equation for the polymer propagator G suitably modified to account for the flow-induced anisotropy in the system. The full macroscopic and microscopic set of equations is solved numerically spectrally. Representative results for the polymer structure, polymer segment concentration and the velocity profile will be presented for 3 cases of polymer solution flows: in the bulk of a rotational viscometric device, above a repulsive surface, and above an adsorbing surface.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

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ΕΡΕΥΝΗΤΙΚΟΥ ΙΝΣΤΙΤΟΥΤΟΥ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ
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ΟΜΙΛΗΤΗΣ : Dr. Octav ENEA, Directeur de Recherche, CNRS Univ. of Poitiers

ΘΕΜΑ : Gas - Phase Processes at Metallized Membranes

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 9 - 5 - 1994

ΩΡΑ : 12.00

ΠΕΡΙΛΗΨΗ : A thin film formed by metallic particles deposited on a Nafion (or ceramic) membrane can be used as an electrode material capable to perform various electrochemical processes in the gas phase at room temperature. The preparation of monometallic or bimetallic deposits and their characterization will be described. Their activity in the oxidation of various organics (alcohols amines, acids,...) will be discussed in relation to their molecular structure and 'intrinsic' properties. Method / Nafion electrodes are very active in the oxidation of hydrogen: some specific phenomena - oscillations, rise of the local temperature - important in fuel cells applications will be examined. A video in English "Searching for a hydrogen electrical vehicle" will present the research performed at A & m University (College Station, Texas) for a hydrid vehicle using both batteries and hydrogen fuel cells.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

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ΕΡΕΥΝΗΤΙΚΟΥ ΙΝΣΤΙΤΟΥΤΟΥ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ
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ΟΜΙΛΗΤΗΣ : Professor Gerald G. Fuller, Chemical Engineering, Stanford University.

ΘΕΜΑ : Optical Rheometry of Complex Liquids

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ Δευτέρα, 9 - 5 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Complex liquids such as polymer melts block copolymers and surfactants, have complex flow behavior as a result of conformational change affected by hydrodynamic forces. The description and prescription of the rheological properties that control these phenomena require the development of accurate constitutive models that properly recognize the distinct microstructure of the many materials that can be encountered. For example in polymer melts the rheology is primarily a result of segmental orientation between entanglements. Surfactants, emulsions and block copolymers, on the other hand, are characterized by structure at a variety of length scales that can dominate flow behavior. Furthermore, many systems are comprised of more than a single constituent and identification of the separate dynamics of each component is often essential to elucidate the mechanisms controlling flow and orientation processes. Optical methods offer important advantages in the measurement of fluid microstructure, and are particularly valuable when made in conjunction with more standard mechanical rheological methods. Because the response can occur over a wide range of length scales, no single optical interaction may uncover all of the important the physical phenomena. In this lecture techniques in optical rheometry are reviewed and their application to a variety of materials is discussed. These techniques include polarimetry measurements of intrinsic birefringence and dichroism, which offer the means of extracting segmental orientation. Scattering dichroism and small angle light scattering are introduced as techniques capable of following larger length scales present in emulsion, surfactants, and polymer blends. Additionally, spectroscopic techniques such as infrared dichroism and polarization modulated Raman scattering are presented and applied to multicomponent systems, such as polymer blends and block copolymers. These spectroscopic methods are shown to allow the dynamics of individual component dynamics to be extracted.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ

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ΟΜΙΛΗΤΗΣ : Professor Thanasis Panagiotopoulos, School of Chemical Engineering, Cornell Univ. Ithaca and Demokritos Research Center, Athens

ΘΕΜΑ : Molecular simulation of strongly associating and reacting fluids

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα 18 - 4 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Strongly associating and reacting fluids are frequently encountered in many chemical and biological applications. Molecular simulation of such systems is challenging because of extreme sampling difficulties. In this presentation, we first discuss a new formalism for calculating the properties of chemically reactive systems, the "Reactive Canonical Monte Carlo" method (Molec. Phys. vol. 81, p. 717, 1994). In this formalism, chemical reactions in the forward and reverse directions are continuously attempted in a way to satisfy chemical equilibrium in a statistical sense. The technique is applied to several strongly associating fluids and the results confirm the validity of Wertheim's theory and are in good agreement with available experimental data for the properties of nitric oxide. Ionic fluids are discussed next, with emphasis on a recently completed calculation of the phase behavior of the restricted primitive model for ionic solutions. The calculations utilize cluster moves that allow displacements and transfers of ionic aggregates. The resulting critical parameters are in modest agreement with previous simulation and theoretical results, and imply that previous estimates of the critical properties of molten salts are too high.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

ΤΜΗΜΑΤΟΣ ΧΗΜΙΚΩΝ ΜΗΧΑΝΙΚΩΝ & ΕΡΕΥΝΗΤΙΚΟΥ ΙΝΣΤΙΤΟΥΤΟΥ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ ΚΑΙ ΧΗΜΙΚΩΝ ΔΙΕΡΓΑΣΙΩΝ ΥΨΗΛΗΣ ΘΕΡΜΟΚΡΑΣΙΑΣ

ΟΜΙΛΗΤΗΣ : Αλκιβιάδης Χ. Παγιατάκης, Καθηγητής Τμήματος Χημικών Μηχανικών, Πανεπιστήμιο Πατρών, Ερευνητής ΕΙΧΗΜΥΘ-ΙΤΕ.

ΘΕΜΑ : Καθεστάτα ροής και σχετικές διαπερατότητες κατά τη διαφασική ροή μέσα σε πορώδη σώματα

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 28 - 1 - 1994

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Στόχος αυτής της εργασίας είναι η εξακρίβωση των μηχανισμών της ροής σε κλίμακα πόρων κατά την ταυτόχρονη διοχέτευση δύο υγρών μέσω πορώδους σώματος, καθώς και ο συσχετισμός των μηχανισμών ροής με τη μακροσκοπική συμπεριφορά του συστήματος. Προς τούτο, διεξήχθη μια ευρεία συστηματική παραμετρική μελέτη αυτής της διεργασίας χρησιμοποιώντας ένα γυάλινο δοκίμιο δικτύου πόρων του τύπου θάλαμοι-και-λαιοί. Οι μηχανισμοί της ροής διαπιστώθηκαν με απ' ευθείας οπτικές παρατηρήσεις καθώς και οπτικές μαγνητογραφήσεις μέσω μακροσκοπίου. Οι αντίστοιχες σχετικές διαπερατότητες προσδιορίστηκαν από τις ογκομετρικές παροχές, οι οποίες εκρατούντο σταθερές (ρυθμιζόμενες) μέσω αντλιών τύπου σύριγγας, και τις απώλειες πίεσεως κατά μήκος του δοκιμίου σε έκαστο των δύο υγρών, οι οποίες κατεγράφοντο συνεχώς μέσω συστήματος μετατροπής πίεσεως. Ένα από τα κεντρικά συμπεράσματα είναι ότι η επί 65 έτη κρατούσα αντίληψη (μάλλον υπόθεση) ότι το μη-διαβρέχον υγρό ρέει μόνο μέσω συνεχών διαδρόμων είναι εσφαλμένη. Όπως προκύπτει, σε τρία από τα τέσσερα κύρια καθεστάτα ροής που παρατηρήθηκαν (συγκεκριμένα, κατά τη δυναμική μεγάλων γαγγλίων, τη δυναμική μικρών γαγγλίων, και τη σταγονοειδή ροή) η ροή του μη-διαβρέχοντος υγρού οφείλεται αποκλειστικά στην κίνηση αποκομμένων τμημάτων του υγρού (γαγγλίων, ή σταγόνων). Αυτό το αποτέλεσμα εξηγεί τις ασυνέπειες που παρατηρούνται στη συμβατική θεωρία κλασματικής ροής και καθιστά απαραίτητη μια ριζική επαναπροσέγγιση της θεωρητικής αναλύσεως της διεργασίας. Η παρουσίαση θα κλείσει με την ανάπτυξη ενός εξομοιωτή διαφασικής ροής σε πορώδη σώματα, ο οποίος συμφωνεί με τις πειραματικές παρατηρήσεις, καθώς και επίδειξη μερικών τυπικών υπολογιστικών αποτελεσμάτων.