

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 : Γεώργιος Γεωργίου, Καθηγητής Τμήματος Μαθηματικών
Πανεπιστήμιο Κύπρου

ΘΕΜΑ : Simulations of extrusion instabilities

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 12 - 12 - 95

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : We explore two different mechanisms of extrusion instabilities. These are based on the combination of nonlinear slip with compressibility in the first case and elasticity in the other. We demonstrate that both mechanisms lead to the periodic storage and release of elastic energy, generating oscillations of the pressure drop similar to those observed experimentally in extrusion instabilities.

We consider the time-dependent axisymmetric incompressible extrudate-swell flow of an Oldroyd-B fluid assuming that slip occurs along the wall following a slip equation which relates the shear stress to the velocity at the wall and exhibits a maximum and a minimum. For the integration of the constitutive equation we use the EVSS method. Standard finite elements are used in space and a fully-implicit (Euler backward difference) scheme is employed for the time integration.

Results are presented for the one-dimensional Poiseuille flow and the two-dimensional extrudate-swell flows. Periodic solutions are obtained at fixed volumetric flow rate when an unstable steady-state is perturbed. The amplitude and the period of the oscillations are increasing functions of elasticity and compressibility.

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ΟΜΙΛΗΤΗΣ : Professor Stratis V. Sotirchos, Dept. of Chemical Engineering,
University of Rochester, Rochester, NY 14627, USA

ΘΕΜΑ : Preparation of functionally graded films and coatings by
chemical vapor deposition methods

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 11 Δεκεμβρίου 1995

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Various reaction engineering issues encountered in the preparation of compositionally graded films and coatings by chemical vapor deposition methods will be addressed in this talk. Compositionally graded (or functionally graded according to the prevailing term in the literature) materials are nanocomposite structures that exhibit continual or continuous variation of their composition in one or more directions. They are of interest in a number of applications, but our own interest lies in their use as protective coatings for carbon and ceramic matrix composites in oxidizing, and possibly corrosive, environments. Compositionally graded coatings can bridge the difference that exists between the thermal expansion coefficient of the base material (carbon or ceramic matrix composite) and that of the outer corrosion - or oxidation - resistant, protective layer, and, in this way, lessen and even eliminate the occurrence of cracks during thermal cycling. Experimental results will be presented on a novel method formulated for the preparation of compositionally graded C/SiC coatings, for carbon-carbon composite protection, through chemical vapor codeposition of carbon and silicon carbide from methyltrichlorosilane and hydrocarbon mixtures. Emphasis will be placed on the existence of multiple steady states in this deposition system since this phenomenon, whenever it occurs, imposes limits on the obtainable codeposit compositions.

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ΟΜΙΛΗΤΗΣ : Prof. Michael Nikolaou, Chemical Engineering Dept., Texas
A&M University, College Station, TX 77843-3122

ΘΕΜΑ : *Model Predictive Control:*
Recent Successes and Future Challenges

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 4 - 12 - 95

ΩΡΑ : 19:00

ΠΕΡΙΛΗΨΗ : Model predictive control (MPC) is a technique for computerized process control. It has now become the de facto standard of advanced control in process industries. How does MPC work, why does it enjoy such popularity, and what challenges does it pose?

MPC employs a mathematical model to predict what would happen to the controlled process as a result of future control actions. An MPC system uses that knowledge and process measurements periodically, to implement what it considers the best control action, after solving a constrained optimization problem in real time. While this on-line optimization creates a complex structure, it provides significant flexibility. MPC can cope directly for events such as a stuck control valve or a faulty sensor. Its positive features have earned MPC widespread acceptance by process engineers and operators.

There is a number of reasons why the design of MPC systems with guaranteed properties has long been a formidable challenge. The presence of constraints renders an MPC system, and consequently an entire closed-loop, nonlinear, therefore impossible to analyze using linear control theory. Difficulty is increased by the fact that control action is not computed through a closed-form expression (e.g. a set of algebraic, differential or difference equations) but rather as the repeated on-line solution of a series of optimization problems.

For over a dozen years the design of constrained MPC systems relied mostly on engineering intuition and judgment. Very recently, research groups, including our own, have obtained results that allow the design of MPC systems in a more rigorous manner. Properties such as closed-loop stability, performance, and robustness can now be guaranteed for processes that are modeled by linear or certain classes of nonlinear models. In this talk, I will present an overview of MPC fundamentals as well as our research and application results in this area. Existing challenges as well as possibilities for future developments in MPC and the broader area of computer-aided process engineering will be discussed.

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ΟΜΙΛΗΤΗΣ : Professor George Jackson, Department of Chemistry,
University of Sheffield, Sheffield, S3 7HF, UK

ΘΕΜΑ : Phase Transitions in Dipolar Systems

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τετάρτη, 22 Νοεμβρίου 1995

ΩΡΑ : 19.00

ΠΕΡΙΛΗΨΗ : Contrary to a number of long standing theoretical predictions, recent simulation studies have shown that spherical repulsive dipolar fluids do not exhibit a vapour-liquid phase transition. This rather surprising finding is attributed to the formation of chains of “nose-to-tail” dipoles in the fluid which prevents the necessary clustering required for vapour -liquid phase transitions. In our work we have investigated the possibility of vapour -liquid coexistence for a fluid of hard spherocylinders with central longitudinal, point dipoles using the Gibbs ensemble Monte Carlo technique. The system is characterised by the length to breadth or aspect ratio L/D of the molecule. For systems of dipolar hard spheres, where $L/D=0$, we indeed confirm that the vapour-liquid equilibrium is precluded by the formation of chains. Similarly, no evidence of phase separation is found for elongated dipolar hard spherocylinders with $L/D=1$. Chains also form in this system but with an antiparallel “side-by-side” arrangement. By making the intermolecular energies of the nose-to-tail and antiparallel orientations equal, which corresponds to $L/D=1/4$, vapour-liquid coexistence is observed.

Whilst simple geometry is able to account for liquid crystal phases, many thermotropic mesogens have a permanent dipole moment which greatly influences the phase behaviour. The effect of the position and strength of the dipole on transition densities and structure is of considerable interest. We have also undertaken an extensive Monte Carlo study of simple hard spherocylinders with point dipoles in a variety of positions and orientations to quantify the effect of dipolar interactions on the phase behaviour. In the case of central longitudinal dipoles we find that the nematic phase is destabilised by the presence of the dipole. Preliminary results for central transverse dipoles are also given. The long range interactions present in these systems are treated using the reaction field and Ewald methods. The latter is very computationally expensive for large systems and we have developed efficient parallel PVM code for use on typical workstation clusters or on parallel supercomputers such as the CRAY T3D.

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

ΟΜΙΛΗΤΗΣ : Dr. K. Takehira, Department of Surface Chemistry, National Institute of Materials and Chemical Reaction, Tsukuba Research Center, AIST, 1-1 Higashi, Tsukuba, Ibaraki 305, Japan

ΘΕΜΑ : Solid Electrolyte aided oxidation of Hydrocarbons

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Πέμπτη, 16 Νοεμβρίου 1995

ΩΡΑ : 20:00

ΠΕΡΙΛΗΨΗ : A cell system using yttria-stabilized zirconia (YSZ) as solid electrolyte, e.g. MIYSZIM ϕ (M and M ϕ ; electrodes) was used for the selective oxidation of hydrocarbons. Ethene and propene were partially oxidized to the corresponding oxygenated compounds, acetaldehyde and acrylaldehyde, respectively while but-1-ene gave both methyl vinyl ketone and crotonaldehyde, by oxygen species generate on an inert Au film vis YSZ at 450°C.) Ethane was also partially oxidized to acetaldehyde (Selectivity: 45%), while propane gave propene, ethene, ethane together with a small amount of acrylaldehyde, which increased with increasing the oxygen flux through the YSZ at 475°C) Ethane gave no ethene and ethanol gave acetaldehyde, suggesting that ethane is oxidized to acetaldehyde via alkoxide intermediate. It is likely that an active oxygen species appeared as an atomic oxygen at the triple phase boundary of Au/YSZ/atmosphere and oxidized the alkenes despite the inertness of the Au for dissociative activation of molecular oxygen. When Rh was used as the anode metal, partially oxidized rhodium metal showed remarkable activity for the partial oxidation of methane into synthesis gas by oxygen species transported through the YSZ under 1 atm and at low temperature of 500°C. It is likely that methane was directly oxidized to synthesis gas, not via reforming reaction with H₂O and CO₂, by the adsorbed oxygen species over the Rh anode, which were electrochemically supplied through the YSZ

Partial oxidation of propene to acrylaldehyde was carried out over a MoO₃-Bi₂O₃ catalyst film layered on the Au/YSZ/Ag systems at 450°C and the activity of oxygen species transported through the catalyst was tested. The results revealed that the oxygen atoms bound to molybdenum insert into an allylic intermediate form acrylaldehyde, while bismuth species are responsible for oxygen incorporation and transportation in the catalyst.) Over a scheelite-type molybdate, but-1-ene gave methyl vinyl ketone and crotonaldehyde at 450-475°C under oxygen pumping; oxygen species transported through the catalyst insert into an allylic intermediate to form the oxygenated products, while oxygen species chemisorbed on the catalyst surface from the gas phase accelerate deep oxidation.) The layered catalyst showed a higher activity and, especially, MoO₃ alone showed a 600 times high activity compared to a fixed bed catalyst. MoO₃ cannot transport oxide ions through itself. The thin MoO₃ films were deposited on Au anode by means of vacuum deposition and sputtering method at room temperature or 300°C. Propene oxidation over the MoO₃/Au/YSZ/Ag at 475°C revealed that the film deposited by sputtering method at 300°C showed the highest activity. This film possess a porous morphology composed of the leaf-like crystals with preferential orientation (010) plane parallel to the pore channel and perpendicular to the Au surface. A relatively high step density was observed on the oriented (010) plane of the crystal. The active oxygen species appear at the Au/YSZ boundary, migrate over the MoO₃ crystal surface, and regenerate the active sites at the steps of MoO₃ crystals, resulting in the high activity.)

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ΟΜΙΛΗΤΗΣ : Δρ. Οδυσσέας Κάρταλος, Institut Français du Pétrole BP 311
92506 Reuil Malmaison, France

ΘΕΜΑ : Flow Properties of Thixotropic Fluids

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 30 Οκτωβρίου 1995

ΩΡΑ : 19.00

ΠΕΡΙΛΗΨΗ : A big variety of fluids encountered in different chemical engineering applications is characterized by thixotropy. This is the case of paints, cosmetics, pesticides, drilling fluids, or pharmaceuticals. Understanding and predicting how thixotropic behaviour affects flow properties is of major importance both from the academic and the industrial point of view.

This work focuses on flow properties of clay-polymer systems and is motivated by current problems of the drilling industry. The following topics will be discussed:

- what are the rheometric techniques to be used in order to obtain the relevant intrinsic properties of the material
- how rheological properties are related to physical-chemical parameters of the system
- what are the appropriate constitutive equations to model flow behaviour under transient and steady flow conditions

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ΟΜΙΛΗΤΗΣ : Καθηγητής Μιχάλης Α. Μαυροβουνιώτης, Chemical Engineering Department, Northwestern University, Evanston, IL 60208-3120

ΘΕΜΑ : Computational Construction and Analysis for Complex Reaction Systems

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 16 - 10 - 1995

ΩΡΑ : 19.00

ΠΕΡΙΛΗΨΗ : Complex chemical reaction systems abound in industrial processes, in analytical instruments, and in living systems. Systems with large numbers of components and reactions are often known only in terms of general types of reactions are difficult to generate manually. We will present a computer language for the formal description of general types of reactions. These descriptions are compiled and automatically applied to any set of initial compounds, to generate the complete network of specific chemical reactions. This approach allows qualitative comparisons as well as the automatic generation of mathematical models. Since complex chemical systems usually involve uncertain or incomplete quantitative information, one must make good use of qualitative or structural information and interleave results from a variety of methods - including a combination of theoretical methods and analysis of high-dimensional measurements. We will present methods for the identification of thermodynamic bottlenecks in pathways, estimation of thermodynamic properties of reaction intermediates, and pattern recognition from process measurements.

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- ΟΜΙΛΗΤΗΣ : Robert G. Gilbert FAA, Professor of Chemistry, The University of Sydney, Director, Sydney University Polymer Centre, Sydney, Australia
- ΘΕΜΑ : Rate coefficients in free radical polymerization: Measurement and Meaning
- ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ
- ΗΜΕΡ/ΝΙΑ : Παρασκευή, 6 Οκτωβρίου 1995
- ΩΡΑ : 11.00 π.μ.

ΠΕΡΙΛΗΨΗ : New methods are rapidly emerging so that rate coefficients and mechanisms in free-radical polymerizations can be measured and understood, without the ambiguity that has so often been a problem hitherto. Propagation rate coefficients can be measured using pulsed-laser polymerization; a novel variant of this will be discussed which overcomes problems which previously prevented the method being used for "hot" monomers such as acrylates. Propagation rate coefficients so obtained can be understood and predicted using transition state theory with accurate quantum mechanical computation of the transition state properties. These calculations give quantitative accord with experiment, and reveal that the magnitude of the frequency factor for propagation is dominated by three hindered rotors in the transition state. Since these rotations are influenced by the penultimate unit, this suggests that significant penultimate unit effects are likely in copolymerizations. Termination rate coefficients can be successfully modelled from a knowledge of the diffusion coefficients for oligomeric species as functions of the degree of polymerization and of polymer fraction, taking account of spin effects. The results of these calculations are able to reproduce data which are very sensitive to termination, viz., relaxation rates (using gamma-radiolysis initiation) and instantaneous molecular weight distributions. In each case, comparison between theory and experiment brings to light unsuspected effects, such as inhomogeneities at high conversion in emulsion polymerizations.

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ΟΜΙΛΗΤΗΣ : Paschalis Alexandridis, Physical Chemistry 1.
University of Lund, Sweden,

ΘΕΜΑ : “Αυτο-οργάνωση Αμφίφιλων Συμπολυμερών”

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : 5-9-1995

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : Αμφίφιλα λέγονται μόρια που αποτελούνται από ένα υδρόφιλο και ένα υδρόφοβο (λιπόφιλο) τμήμα. Η διπλή φύση των αμφίφιλων μορίων διευκολύνει την αυτο-οργάνωσή τους όταν βρίσκονται μέσα σε διαλύματα, και προσδίδει μοναδικές ιδιότητες διαμερισματοποίησης (π.χ. κυτταρική μεμβράνη) ή ομοιογενοποίησης (π.χ. γαλακτώματα). Ο έλεγχος κατά τον πολυμερισμό της χημικής σύστασης και του μοριακού βάρους, οδηγεί στη σύνθεση αμφίφιλων κατά συστάδες συμπολυμερών με διαφορετικές υδρόφιλες-λιπόφιλες ιδιότητες και τρόπο αυτο-οργάνωσης. Τα συμπολυμερή αυτά είναι έτσι κατάλληλα για ποικίλες πρακτικές εφαρμογές (π.χ. απορρυπαντικά, καλλυντικά, φάρμακα, τρόφιμα κ.λ.π.). Η αυτο-οργάνωση αμφίφιλων συμπολυμερών του τύπου πολυ(αιθυλενοξειδίου)-πολυ(προπυλενοξειδίου) (PEO-PPO) σε υδατικούς διαλύτες και μίγματα νερού-ελαίων αποτελεί το θέμα της διάλεξης. Τα μόρια του συμπολυμερούς, με αύξηση της συγκέντρωσης τους σε νερό, αυτο-οργανώνονται σε σφαιρικά μικύλλια, τα οποία, με περαιτέρω αύξηση της συγκέντρωσης του πολυμερούς, (α) κρυσταλλώνονται σε κυβικές δομές, (β) επιμηκύνονται και σχηματίζουν κυλίνδρους με εξαγωνική δομή και (γ) τοποθετούνται κατά στρώματα. Σταδιακή αντικατάσταση του νερού (καλός διαλύτης για το τμήμα PEO) με οργανικό διαλύτη (καλός για το τμήμα PPO) οδηγεί στο σχηματισμό ανάστροφων δομών. Η επίδραση του μοριακού βάρους, του μεγέθους των τμημάτων PEO-PPO, και της θερμοκρασίας στο τρόπο αυτο-οργάνωσης των αμφίφιλων συμπολυμερών παρουσιάζεται στη διάλεξη, και η αυτο-οργάνωση των συμπολυμερών σε μίγματα νερού-οργανικού διαλύτη συγκρίνεται με την αντίστοιχη αυτο-οργάνωση κατά συστάδες συμπολυμερών που παρατηρείται σε τήγματα.

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ΟΜΙΛΗΤΗΣ Dr. Kostas N. Christodoulou, DuPont Central Research and Development, Experimental Station, Wilmington, DE 19880

ΘΕΜΑ : Operability and stability of viscous free surface flows

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Παρασκευή, 7 Ιουλίου 1995

ΩΡΑ : 19.00

ΠΕΡΙΛΗΨΗ : The stability of two-dimensional (2D), steady, viscous free surface flows to small, 2D and 3D disturbances is analyzed by the Galerkin/finite element method and linear stability theory. Disturbances are expanded in Fourier modes in the third dimension and the same basis functions are used to represent the two-dimensional dependence as the base flow. The linearized residuals of the Navier-Stokes systems that governs the 3D unsteady flow reduce to a large, asymmetric generalized eigenproblem. By the deflated Arnoldi algorithm and a matrix transformation, the most dangerous modes and their growth rates are calculated, without any simplifications, as functions of flow parameters and disturbance wavenumber. Critical values of parameters and wavenumber are tracked directly as additional flow parameters are changed, by solving extended systems to establish operability diagrams in two-parameter spaces. Frequency response analysis to 3D disturbances establishes optimum operating conditions, so-called quality windows, within the operability limits. The methods of analysis are tested against published results on the stability of a stagnant liquid layer, Hele-Shaw flow, and flow between counter-rotating rollers (forward roll coating). They are applied to slide coating flow, a more complex flow, involving both static and dynamic wetting lines. Loss of stability resulting in flooding, meniscus break-up, spontaneous oscillations (barring) and bifurcations to 3D (ribbed) states are uncovered. Finally, the shape and rheology of a multilayer side coating system are optimized for maximum operating latitude.



FOUNDATION FOR RESEARCH AND TECHNOLOGY-HELLAS

INSTITUTE OF CHEMICAL ENGINEERING
AND HIGH TEMPERATURE CHEMICAL PROCESSES

P.O. BOX 1414, GR - 265 00 PATRAS, GREECE

July 6, 1995

This is to certify that I received an honorarium of 30.000 Drs. for giving the seminar titled:

**"Relaxation and Difussion
in Amorphous Materials and Glas-forming Liquids"**

to the Institute of Chemical Engineering and High Temperature Chemical Processes.

Name: **Dr. K.L. Ngai**

Signature: *K.L. Ngai*

Date: *July 6th 1995*

Passport No.: *014058948*

Address: *9516 Woody Lane*

Great Falls

VA. USA 22066

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ΕΡΕΥΝΗΤΙΚΟΥ ΙΝΣΤΙΤΟΥΤΟΥ ΧΗΜΙΚΗΣ ΜΗΧΑΝΙΚΗΣ ΚΑΙ
ΧΗΜΙΚΩΝ ΔΙΕΡΓΑΣΙΩΝ ΥΨΗΛΗΣ ΘΕΡΜΟΚΡΑΣΙΑΣ

ΟΜΙΛΗΤΗΣ : Professor Gary L. Haller, Department of Chemical Engineering,
Yale University, P.O. Box 208286, New Haven, CT 06520-8286.
USA

ΘΕΜΑ : Physical and Chemical Characterization of Mesoporous
Molecular Sieve Materials

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων

ΗΜΕΡ/ΝΙΑ : Δευτέρα, 15 Μαΐου 1995

ΩΡΑ : 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : The mesoporous molecular sieves (MCM-41) recently discovered by Mobil are potentially interesting catalysts and catalyst supports [1]. These materials have uniform parallel channels in the range of 15-100Å. We have prepared a series of these materials with five Si/ Al ratios (0.7, 1.1, 3.0, 5.0 and 16) with six pore sizes between 15-40Å. We have characterized these materials by small angle IR, XRD, TEM, ^{27}Al , ^{29}Si MAS NMR. The crystallinity, porosity and acidity are functions of the source of the pseudobornemite used in the preparation and of the pore size which was varied by the alkyl chain length of the alkyl trimethyl ammonium template used (C_6 , C_8 , C_{12} , C_{14} and C_{16}). It is possible to prepare precursors with only tetrahedral Al up to about 20 wt% alumina for all pore sizes. However, after calcination, only the smallest pore sieve retains all of the alumina in a tetrahedral environment. For chemical characterization, we have used hydrocarbon adsorption and two acid catalyzed reactions, cumene hydrogenolysis and 2-methyl - 2 - pentene isomerization. To first order, the acidity measured by the initial rate of methyl shift in 2-methyl-2-pentene, correlates with the fraction of alumina in tetrahedral sites, in detail, the variation of acidity is a more complex. For example, a maximum in acidity is found at a Si/ Al ratio of three (at constant pore size of 37Å) and a minimum in acidity is observed at a pore size of 25Å (at constant Si/ Al ratio of 16). The complete grid of structural changes determined by ^{27}Al and ^{29}Si NMR and acidity determined by -2-methyl-2-pentene will be presented. The correlation between structure and acidity will be interpreted in terms of variation of bond length and bond angle which are not a unique function of either composition or pore size, but determine the overall acidity of the structure.

[1]. C.T. Kresge, M.E. Leonowicz, W.J. Roth, J.C. Vartuli and J.S. Beck, Nature, 359, 710 (1992).

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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ΟΜΙΛΗΤΗΣ : E. Manias, Department of Polymer Science & Materials Science
Centre, University of Groningen, The Netherlands

ΘΕΜΑ : Tribology at the Molecular Scale

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ Δευτέρα 8 Μαΐου 1995

ΩΡΑ 7.00 μ.μ.

ΠΕΡΙΛΗΨΗ : The understanding of wear, friction, lubrication and adhesion is essential for the development of new materials and devices. Given the ever increasing miniaturization in technology, the scientific interest has shifted towards the study of the behaviour of nanoscale systems. Recent rapid progress in experimental methods, such as the Atomic Force Microscope (AFM) and the Surface Forces Apparatus (SFA) provide the researchers the ability to experimentally study and reveal a very rich and often striking behaviour at the nanometer length scale. These kinds of experiments are very naturally complemented by computer simulations such as Non-Equilibrium Molecular Dynamics (NEMD). A multidisciplinary approach, introducing the above experimental and computational techniques and comparing experimental and simulation findings, will focus on the study of nanoscopically confined oligomer films under shear.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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

ΟΜΙΛΗΤΗΣ : Dr. Theodoros Karapiperis, Paul Scherrer Institute, Switzerland

ΘΕΜΑ : Cellular Automation Model of Coupled Mass Transport and Chemical Reaction

ΤΟΠΟΣ : Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ : Τρίτη, 2 Μαΐου 1995

ΩΡΑ : 19.00

ΠΕΡΙΛΗΨΗ : Mass transport coupled with chemical reactions, is modelled as a cellular automaton in which solute molecules perform a random walk on a regular lattice and react according to a local probabilistic rule. Stationary solid particles dissolve with a certain probability and, provided solid is already present and / or the solution is saturated, solute particles have a probability to precipitate. No a priori restriction is placed on the number of particles per lattice site. Assuming molecular chaos and a smooth spatial dependence of particle density, we obtain, in the continuum limit, the macroscopic reaction-transport equations with standard advection, diffusion and reaction terms.

The model is first applied to homogeneous systems subject to the reactions $a+b \leftrightarrow c$ and $a+b \rightarrow c$. In the reversible case we find that correlations between diffusing reactants can influence the macroscopic properties of the equilibrium state. In the case of the irreversible reaction, the decline of reactant density is slowed down because of density fluctuations that lead to segregation of the reactants; the time dependence of the density is found to follow asymptotically a different power law from that obtained from the rate equation; compared to pure diffusion, reaction elimination proceeds faster and follows a different asymptotic law when there is relative advection between a and b . In the simulation of an initially separated $a+b \rightarrow c$ system, the width of the reaction zone is found to grow faster than predicted by the reaction - diffusion equations.

We also simulate autocatalytic reaction schemes displaying spontaneous formation of spatial concentration patterns. In particular we apply our model to the Brusselator, as well as to the Selkov and Schackenberg reaction schemes.

Our simulation of the dissolution of a solid block in a streaming fluid yields solid precipitation downstream from the original solid edge, in contrast to the standard reaction-transport equations. The additional precipitation of solid is accompanied by a substantial reduction in the relatively small solute concentration. The observed effect is the result of fluctuations in solute density and varies according for the study of the role of intrinsic fluctuations in the presence of reaction threshold and can be employed to investigate porosity changes associated with the carbonation of cement.

Σ Ε Μ Ι Ν Α Ρ Ι Ο

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ΟΜΙΛΗΤΗΣ Dr. Fritz Kalhammer, Vice President, U.S. Electric Power Research, Institute (EPRI), Palo Alto, CA 94303

ΘΕΜΑ The Exploratory Research Program of the U.S. Electric Power Research Institute

ΤΟΠΟΣ Αίθουσα Σεμιναρίων ΤΧΜ

ΗΜΕΡ/ΝΙΑ Δευτέρα, 17 - 4 - 1995

ΩΡΑ : 6.00 μ.μ.

ΠΕΡΙΛΗΨΗ : The Electric Power Research Institute (EPRI) represents the collaborative R&D investment of the majority of the electric utilities in the United States. With the financial support and strategic guidance provided by utilities, EPRI plans, designs, funds and manages one of the world's largest and most diverse private (non-government) energy - and electricity - related R&D programs.

While most of EPRI's R&D is addressing the near-term issues of its member utilities, about 15% of the Institution's funds are used to support research with longer-term objectives. Under the umbrella of Strategic Research and Development (SR&D), this research to overcome fundamental barriers to major advances in energy technology, to explore the feasibility of new concepts with relevance to some aspect of electricity, and exploit opportunities emerging from recent scientific discoveries. SR&D currently funds approximately 200 projects in the Physical (including Chemical), Engineering Materials, Biological & Environmental and Mathematical & Information Science. More than half of the projects are performed by principal investigators at universities, mostly in the U.S.

The major strategic goals driving the programs of EPRI and SR&D will be discussed briefly, and examples of promising research directions and results will be given, with emphasis on research in chemistry and electrochemistry.