



Research in Transport Phenomena

John Tsamopoulos



Plasma Technology Group



Prof. D. Mataras



Assist. Prof. E. Amanatides

www.plasmatech.gr

Laboratory of Applied Mathematics



Prof. G. Dassios



Assist. Prof. P. Vafeas

Laboratory of Transport Phenomena and Physicochemical Hydrodynamics



Assist. Prof. Ch. Paraskeva

Laboratory of Statistical Thermodynamics and Macromolecules



Prof. V. Mavrantzas



Laboratory of Computational Fluid Mechanics



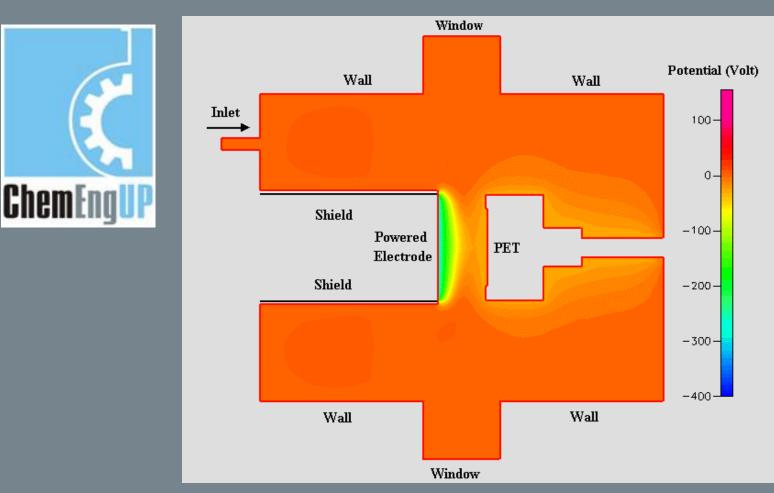
Prof. J. Tsamopoulos



Assist. Prof. Y. Dimakopoulos

http://fluidslab.chemeng.upatras.gr

Research Groups



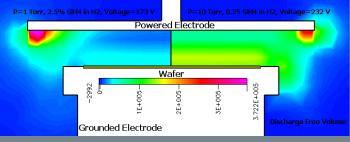
Plasma Technology Laboratory

Simulation of Plasma Processes Development of self-consistent fluid and hybrid models for PECVD of thin films

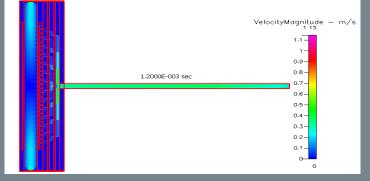
Research Activities in transport phenomena

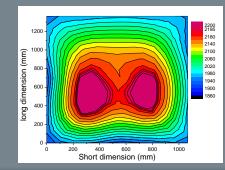
- Development of self-consistent fluid and hybrid models for PECVD of thin films (silicon thin films, Diamond Like Carbon)
- Plasma reactors modeling (flow, heat and mass transfer, gas and surface chemistry, electromagnetics) for new designs or improvement of already existing systems
- Investigate mechanisms of nanostructures growth and deposition uniformity

Plasma voltage during RF cycle



Powered electrode design





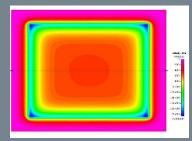
Map of film thickness in large – area reactor

Research Activity: Self-consistent plasma models

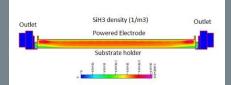
The problem: PECVD simulators do not include electromagnetic problem and film growth. Insufficient to study Deposition Uniformity in Large Area Thin Film Silicon Photovoltaics

Modeling procedure in PTL

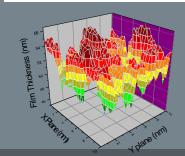
- Step 1: Include Maxwell equations and EM propagation in large area plasma reactors
- Step 2: Couple Maxwell equations with electron and ions kinetics
- Step 3: Gas phase kinetics: Transport and Chemistry
- Step 4: Couple plasma and EM simulator with kMC code for modeling of film growth and structure! (in collaboration with the group of Prof. V. Mavrantzas)



Electric field distribution in large area RF electrode



Map of Reactive Species distribution in SiH₄/H₂ plasmas



Calculated silicon thin film morphology and structure (kMC code)

Develop for 1st time a global PECVD simulator for small and large area reactors Support design of reactors for large area (1.4x1.1m) deposition of silicon EU FP7- "PEPPER project" 2010-2013, 11M€ total, ~1M€ for PTL



Total budget (2007-2013) 1.18M€, 2 European, 2 Industrial projects FP6 IP – "Advanced Thin Film Technologies for Cost Effective Photovoltaics (ATHLET)" 2006-2010, 280k€

- UPAT ARCHER "Simulation of an industrial scale PECVD reactor for deposition of thin film solar modules", Industrial project 2011-2013, 71k€
- UPAT AEC Inc" Simulation of Low Pressure Chemical Vapor Deposition Reactor for deposition of ZnO thin films", Industrial project 2011-2012, 12k€
- EU FP7 "Demonstration of high performance Processes and equipment for thin film silicon photovoltaic modules produced with lower environmental impact and reduced cost and material use", 2010-2013 850k€

ChemEngler Publications, Conferences, Patents

Publications 2007-2013: 35, References (excluding self-ref): 560, Conference Proceeding and presentations: 62

1. "A hybrid kinetic Monte Carlo method for simulating silicon films grown by plasma-enhanced chemical vapor deposition" D.G. Tsalikis, C. Baig, V.G. Mavrantzas, E. Amanatides and D. Mataras Journal of Chemical Physics, Accepted Corrected Proofs (2013)

2. "Growth kinetics of plasma deposited microcrystalline silicon thin Flms", E. Amanatides and D. Mataras, Surf. Coat. Technol., 205 178 (2011)

3. "Simulation of cylindrical electron cyclotron wave resonance argon discharges", S. Sfikas, E. Amanatides, D. Mataras and D.E. Rapakoulias, J. Phys. D - Appl. Phys., 44 165204 (2011)

4. "Fluid Model of an Electron Cyclotron Wave Resonance Discharge", S. A. Sfikas, E. K. Amanatides, D. S. Mataras and D. E. Rapakoulias, IEEE Trans. Plasma Science 10.1109/TPS.2007.905946 Page(s): 1420-1425 (2007)

5. "Simulation of The Electrical Properties of SiH4/H2 RF Discharges", B. Lyka, E. Amanatides and D. Mataras, Jap. J. Appl. Phys. 45 8172-8176 (2006)

6. "Relative importance of hydrogen atom flux and ion bombardment to the growth of μ c-Si:H thin films", B. Lyka, E. Amanatides and D. Mataras, Journal of Non-Crystalline Solids, 352 1049 (2006)

7. "Plasma 2D modeling and diagnostics of DLC deposition on PET", E. Amanatides, P. Gkotsis, Ch. Syndrevelis and D. Mataras, Diamond and Related Materials, 15 904 (2006)

8. "Plasma Enhanced Chemical Vapor Deposition of Silicon under Relatively High Pressure Conditions", E. Amanatides, B. Lykas and D. Mataras, IEEE Trans. Plasma Sci. 33, 372 (2005)



1 Professor, 1 Assistant Professor, 1 Lecturer, 1 PostDoc, 1 PhD Student, 2 diploma thesis students



D. Mataras, Prof.



E. Amanatides Assist. Prof



N. Spiliopoulos Lect.(Physics Dept.)

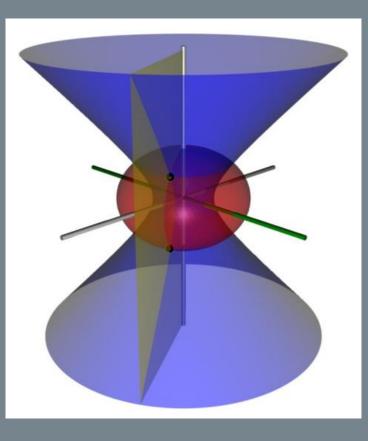


S. Sfikas PostDoc



G. Tsigaras PhD





Laboratory of Applied Mathematics

George Dassios, Professor, and Panagiotis Vafeas, Assistant Professor

Applied Mathematics

Laboratory of Applied Mathematics

Description and Goals

- Motivation: demand for the introduction of realistic models to the mathematical study of phenomena associated to Science and modern Technology.
- Purpose: promote teaching and research in the development and analysis of methods related to Mathematical Physics.



- Partial differential equations. Applications to physical problems using analytical and hybrid methods or purely numerical techniques.
- B.V.P. in ellipsoidal geometry and their applications.
- Radiation, wave propagation and scattering in the fields of Acoustics, Electromagnetism, Elasticity and Thermoelasticity.
- Inverse scattering problems in the above physical areas and development of solution methods.
- Methods of Medical Imaging. Applications to Electroencephalography, Magnetoencephalography and Ultrasonics.
- Fluid Dynamics and in particular Stokes Flow (creeping flow). Conductive and non-conductive magnetic fluids. Micropolar flow with applications to Magnetohydrodynamics and Ferrohydrodynamics.



Main Contributions in Brain Imaging

- Electroencephalography (EEG) can recover no more than 1/3 of the activated neuronal current.
- Magnetoencephalography (MEG) can recover no more than 2/3 of the activated neuronal current.
- Synchronous EEG and MEG recordings still leave the 1/3 of the neuronal current unidentifiable.
- EEG and MEG analysis in realistic ellipsoidal geometry of brain— —head system. Image systems for ellipsoidal harmonic fields.

Main Contributions in Medical Physics

- Growth of ellipsoidal tumors.
- Early tracking of developing brain edema.

Application: Scattering Theory and Stokes Flow

Main Contributions in Scattering Theory

- Low—frequency scattering (also in ellipsoidal geometry):
 - Acoustics.
 - Electromagnetism.
 - Elasticity.
 - Thermoelasticity.
 - Anisotropic media.
 - Tensorial wave fields.

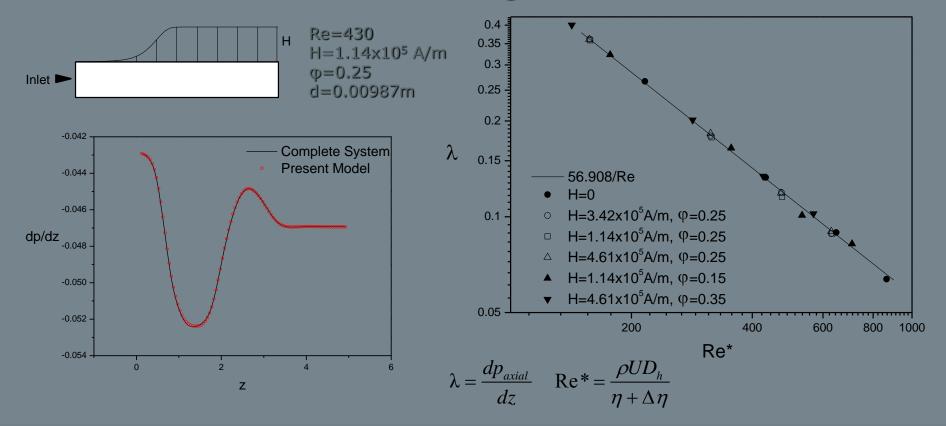
Main Contributions in Stokes Flow

- Introduction of the semi–separable solutions for boundary value problems.
- Flows in ellipsoidal geometry.
- Invariant nonlinear transformations.



Numerical Implementation

Axial pressure gradient and resistance coefficient of ferrofluid in a non-constant transverse magnetic field

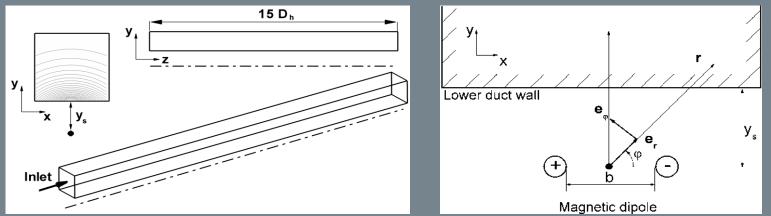


Applied Mathematics

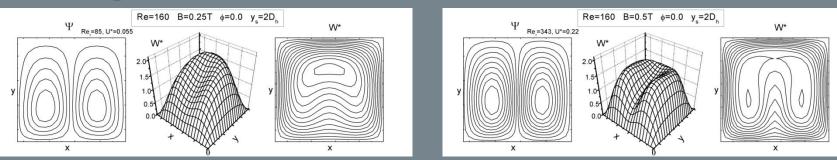


Square Duct Flow

Duct and magnetic field configuration



Stream function Ψ, normalized axial velocity w* and contours for magnetic fields B=0.25T and B=0.5T



Applied Mathematics



Funding

- Program BRAIN: Marie Curie Chair of Excellence at the DAMTP of the University of Cambridge (2005–2008).
- Program K. Karatheodori: "Mathematical and computational development of 3–D models for the magnetohydrodynamic flow of magnetic fluids" (2010–2013).

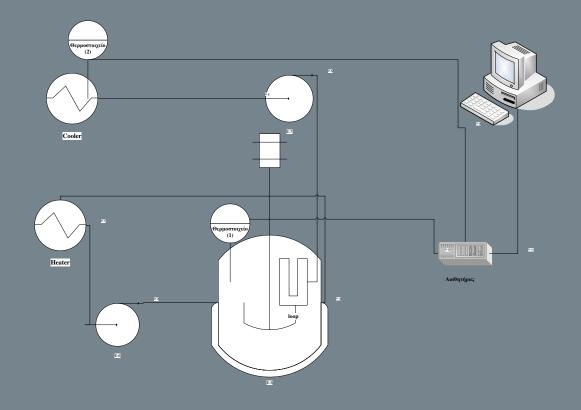
Publications

- Book: *Ellipsoidal Harmonics*, Cambridge University Press (2012) (the first in the field).
- Parsopoulos, K.E., Kariotou, F., Dassios, G., Vrahatis, M.N., Tackling magnetoencephalography with particle swarm optimization". (2009) International Journal of Bio-Inspired Computation 1 (1-2), pp. 32-49
- P.M. Hatzikonstantinou and P. Vafeas "A general theoretical model for the magnetohydodynamic flow of micropolar magnetic fluids. Application to Stokes flow", Mathematical Methods in the Applied Sciences (Math. Methods Appl. Sci.), 33, 233–248 (2010).
- G. Perrusson, P. Vafeas and D. Lesselier, "Low–frequency dipolar excitation of a perfect ellipsoidal conductor", Quarterly of Applied Mathematics (Quart. Appl. Math.), 68, 513–536 (2010).
- P.K. Papadopoulos, P. Vafeas and P.M. Hatzikonstantinou, "Ferrofluid pipe flow under the influence of the magnetic field of a cylindrical coil", Physics of Fluids (Phys. Fluids), 24 (122002), 1–13 (2012).
- G. Dassios, F. Kariotou and P. Vafeas, "Invariant vector harmonics. The ellipsoidal case", Journal of Mathematical Analysis and Applications (J. Math. Anal. Appl.), 405, 652–660 (2013).



- George Dassios (Professor Emeritus)
- Panayiotis Vafeas (Assistant Professor)
- Michael Doschoris (Post Doctorate Researcher)
- Konstantia Satrazemi (Ph.D. Candidate)
- Vasiliki–Christina Panagiotopoulou (Ph.D. Candidate)





Laboratory of Transport Phenomena and Physicochemical Hydrodynamics

Christakis Paraskeva, Assistant Professor

Recovery Of Phenolic Compounds

REMOVAL AND RECOVERY OF PHENOLIC COMPOUNDS FROM OLIVE MILL WASTEWATER BY COOLING CRYSTALLIZATION

Problem

 Olive Mill Wastewater is classified as a hardly degradable waste because of the high organic loading and the content of elevated concentration levels of phenolic compounds.

• The disposal of untreated OMW into aquatic receptors occur environmental consequences such as water contamination, eutrofication, odor and aesthetic deterioration.

Motivation

Phenolic compounds are among, the most complex and the most difficult to remove compounds from the by-products of olive mill wastewaters (OMW).
On the other hand, due to significant properties, including stability and anti-oxidative activity, the recovery of poly-phenols from OMW is of paramount importance and today, are considered as byproducts with high added value (e.g. the phenol hydroxytyrosol costs 6 Euros/mg)

Scope of the current work

Isolation and removal of phenols from olive mill wastewaters based on a cooling crystallization process



IDEA:

The imposed temperature difference in the system results to a concentration difference sufficient for the formation of crystals on the cold surface.



 $t = 30 \sec \theta$

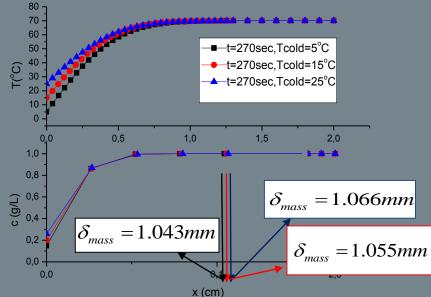
 $t = 1 \min$

 $t = 5 \min$

Crystal precipitation and growth of a phenol takes place immediately upon immersion of the cooling surface in the respective solution.

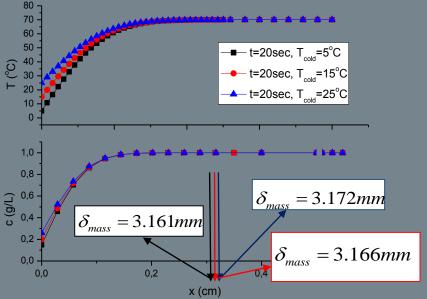
Recovery Of Phenolic Compounds





crystallization

0.2 0,0 x (cm) Conduction: Calculated concentration profile of trans-cinnamic acid for various temperatures Tcold in the reactor past t=270 sec from the onset of



Convection: Calculated concentration profile of trans-cinnamic acid for various temperatures Tcold in the reactor past t=20 sec from the onset of crystallization



Project:

PANELEA: A cost effective system development for complete exploitation of olive mill wastewater, (CEU/CRAFT, Regional, Innovation Poles, GGET, Development of sustainable solutions for the management of olive mill wastewaters with emphasis on the valorization of by-products, 2006-2009

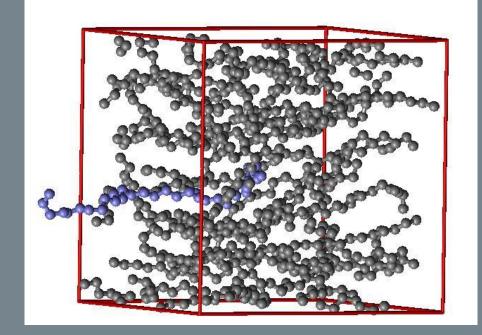
Publication:

_Spyridon S. Kontos, Petros G. Koutsoukos, Christakis A. Paraskeva, 'Removal and recovery of phenolic compounds from olive mill wastewater by cooling crystallization", in Journal of Crystal Growth

Researchers

- Petros Koutsoukos (Professor)
- Christakis Paraskeva (Assistant Professor)
- Spyros Kontos (Ph.D. Candidate)





Laboratory of Statistical Thermodynamics and Macromolecules

Vlasis Mavrantzas, Professor



- Develop reliable, thermodynamically admissible constitutive models for polymer melts and solutions

 Generalized bracket [Beris Edwards, 1994]
 GENERIC (Grmela Öttinger, 1998]
- 1) Parameterize these models on the basis of atomistic simulation results for model systems
- Employ the models to large-scale numerical calculation of polymer flows of interest in the industrial processing of polymer fluid



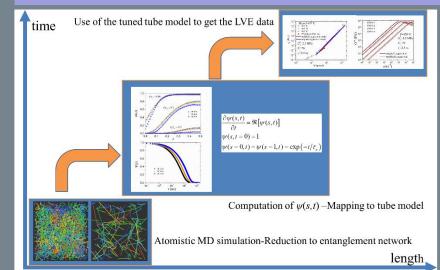
- Project 1: Formulate improved constitutive equations for high-MW homopolymer and bidisperse polymer melts
 - Independently execute Molecular Dynamics Simulations
 - Map the outcome of these simulations onto the reptation model
 - Provide improvements or refinements to the model
 - Compare extensively with experimentally measured viscoelastic data
- Project 2: Extend method to polymer nanocomposites (PNCs)

Non-Equilibrium Thermodynamics formalisms

$$\frac{\partial F}{\partial t} = \{F, H\} + [F, H]$$
Generalized
Bracket

$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{L} \cdot \frac{\delta E}{\delta \mathbf{x}} + \mathbf{M} \cdot \frac{\delta S}{\delta \mathbf{x}} \quad \text{GENERIC}$$

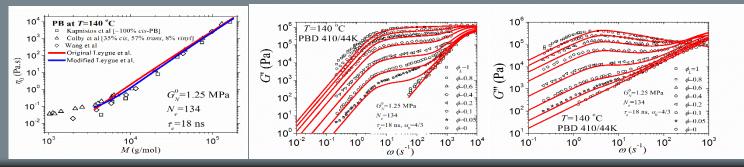
Multi-scale methodology





Multi-scale modeling of polymer melt viscoelasticity: From atoms, to molecules, to primitive paths, to tube models

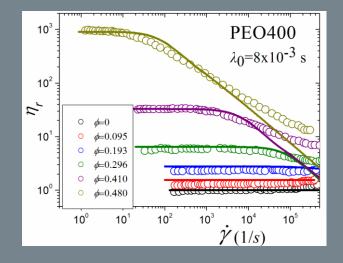
- Goal: Derive the spectrum of the linear viscoelastic (LVE) properties of high-MW polymer melts (homo- and bidisperse) by mapping the outcome of MD simulations onto the tube model
- Method:
 - First map atomistic trajectories to trajectories of primitive paths (PPs) for moderately entangled polymers of a given chemistry
 - Use the latter to parameterize a reliable molecular model for polymer dynamics. We chose the reptation theory based on the tube model – Key ingredient to compute: the so called PP segment survival probability function $\psi(s,t)$
 - We even suggest changes to the functional form of the model or its boundary conditions
 - Use the new model to predict the LVE properties of the same polymer chemistry but of significantly higher MW





A differential constitutive equations for PNCs based on principles of non-equilibrium thermodynamic

- PNCs are formed by the addition of nanoparticles (NPs) to a polymer matrix. They typically exhibit significantly improved properties relative to the pure polymer matrix even at extremely small volume fractions (loadings) of the fillers
- Goal: Develop a thermodynamically-admissible model that can account for:
 - The intriguing phase separation of PNCs
 - Their complex rheology even for spherical NPs
 - Tool: The Generalized bracket formalism by Beris-Edwards.
- Result: A new constitutive model that can accurately describe:
 - the phase behavior of PNCs (swelling of polymer chains by NPs)
 - Their shear rheology (see figure on the right)





- Stephanou P.S., V.G. Mavrantzas, "Quantitative predictions of the linear viscoelastic properties of entangled polyethylene and polybutadiene melts via modified versions of modern tube models on the basis of atomistic simulation data", J. Non-Newt. Fluid Mech. 2013, 200, p. 111.
- Qin J., S.T. Milner, P.S. Stephanou, V.G. Mavrantzas, "Effects of tube persistence length on dynamics of mildly entangled polymers", J. Rheology 2012, 56, p. 707.
- Stephanou P.S., C. Baig, V.G. Mavrantzas, "Toward an improved description of constraint release and contour length fluctuations in tube models for entangled polymer melts from detailed atomistic molecular dynamics simulation data", Macromol. Theory & Simul. 2011, 20, p. 752.
- Stephanou P.S., C. Baig, V.G. Mavrantzas, "Projection of atomistic simulation data for the dynamics of entangled polymers onto the tube theory: Calculation of the segment survival probability function and comparison with modern tube models", Soft Matter 2011, 7, p. 380.
- Baig C., V.G. Mavrantzas, H.C. Öttinger, "On Maxwell's Relations of Thermodynamics for Polymeric Liquids away from Equilibrium", Macromolecules 2011, 44, 640.



- THALES 2012 (National): Graphene and its nanocomposites: Production, properties and applications
 - LSTM Budget: 30 kEuro
- EC-FP7: Multi-scale modeling of interfacial phenomena in acrylic adhesives undergoing deformation (MODIFY)
 - Partners: Upatras (coordinator), DOW, LBI, ETH-Z, UCL, CNRS, ESPCI, MIT, Utokyo,
 - LSTM budget: 402.3 kEuro
- DOW Chemicals Industrial project II: Multi-scale simulation of polyethylene melt rheology and processing properties
 - LSTM Budget: 75 kEuro



1 Professor, 1 PostDoc

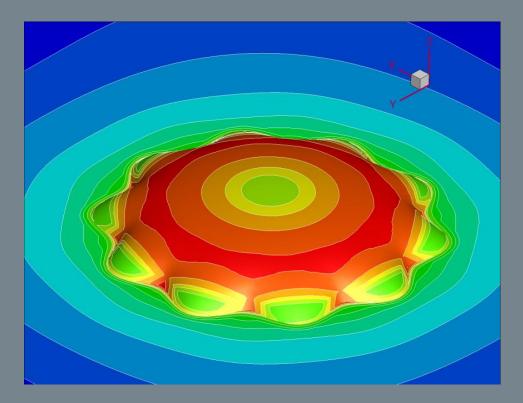


Vlasis Mavrantzas, Prof.



Dr. Pavlos S. Stephanou





Simulation of complex & biological flows

John Tsamopoulos, Professor and Yannis Dimakopoulos, Assistant Professor*

Appointment Pending

Simulation of complex & biological flows



- Computational Fluid Mechanics and Transport Phenomena
- Computational Rheology
- Rheological Modeling
- Bubble Dynamics
- Biological Flows
- Cardiovascular Modeling
- Large Scale Computations



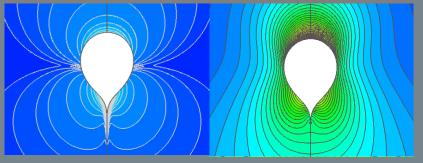
Research Activities: Bubble Dynamics

Rising Bubbles in complex fluids

Applications

- Entrapment of air bubbles in many foodstuffs to improve their flavor and texture (i.e. chocolate, ketchup)
- Prevention of large bubble formation in drilling mud, which may cause dangerous explosions, inhibit production and potentially inflict huge burden on the ecosystem and the finances of oil-drilling companies

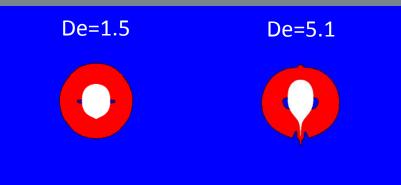
Stress field around a cusped bubble rising in a Polymeric Solution



Effect of De on yield surfaces and shapes of a bubble rising in an elasto–viscoplastic Fluid (Carbopol). The yielded area is in red.

Issues under investigation

- Calculate velocity discontinuity conditions and bubble shapes in polymer solutions
- Calculate entrapment conditions in elastoviscoplastic fluids





Pulsating Bubble

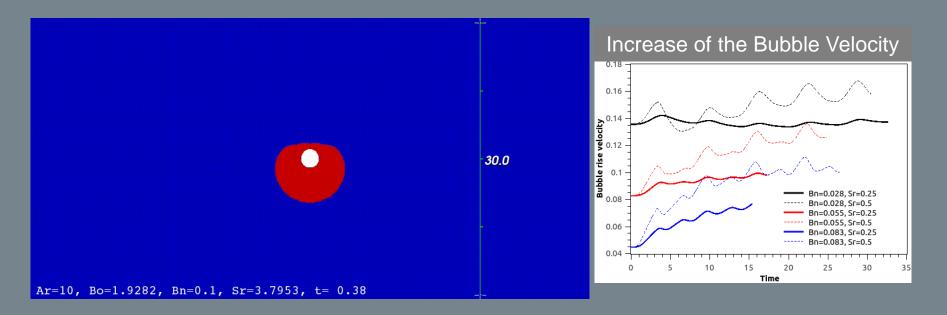
Applications

bubble removal from structural (i.e. cement) through vibration

$$P_{\infty} = P_{ls} + \varepsilon \sin(\omega_f t)$$

Issues under investigation

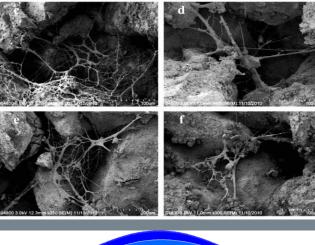
 Predict the optimum parameters of the acoustic field leading to maximization of the increase in the bubble rising velocity.

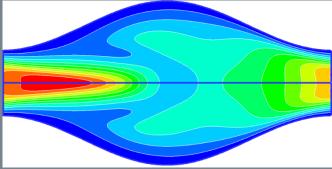




Research Activities: Complex Flows

J. Petrol. Sc. & Engrg, 90-91 (2012)





polymer migration in porous media

Applications

Polymer is added to water to increase the mobility ratio and improve reservoir sweep efficiency and water shut-off technologies

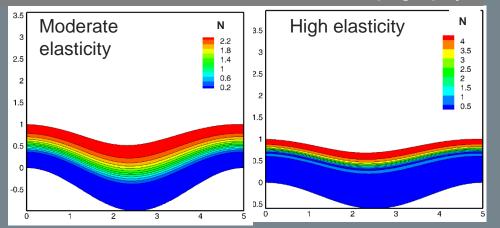
Issues under investigation

Examine how distribution of macromolecules in porous media is affected by flow and physical properties in single phase flows

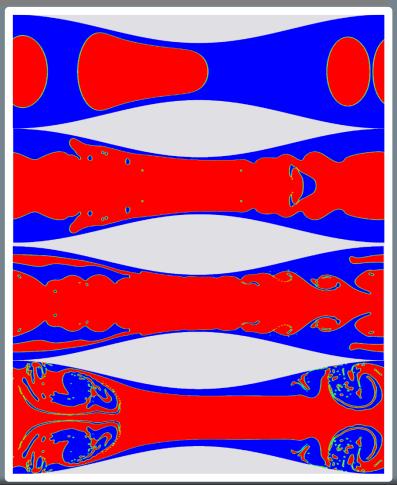
Research Activities: Complex Flows

Variation of polymer concentration in ... single Phase Flow inside an undulating tube

 $\int_{a}^{b} \frac{Small}{amplitude} \int_{a}^{b} \frac{Small}{b} \int_{a}^{b} \frac{$



Effect of increasing the flow rate on the flow patterns of two immiscible fluids in an undulating tube

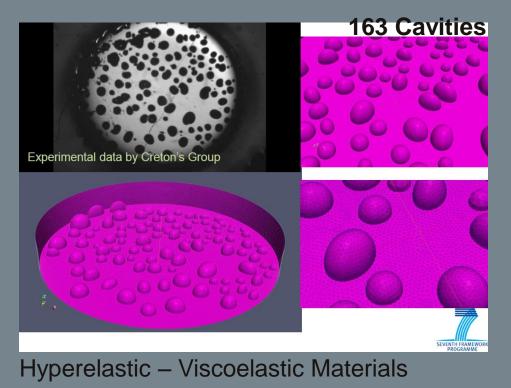


Simulation of complex & biological flows



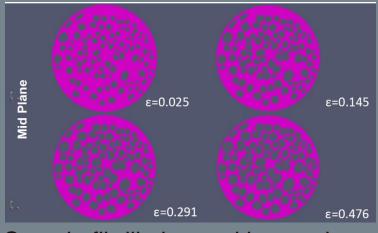
Research Activities: Complex Materials Large Scale Simulations

Mechanical testing of Pressure Sensitive Adhesives - PSAs



PSAs were studied in the EU-funded project "MODIFY" aiming at building fundamental understanding of the role of material structure and properties in their performance.

- 3D & Parallel Computations
- Homemade codes



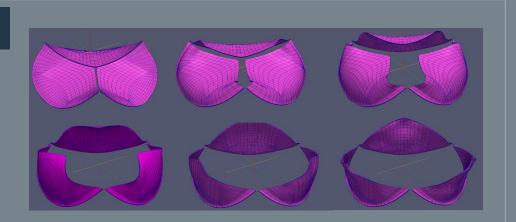
Sample fibrillation and interaction of cavities

Simulation of complex & biological flows



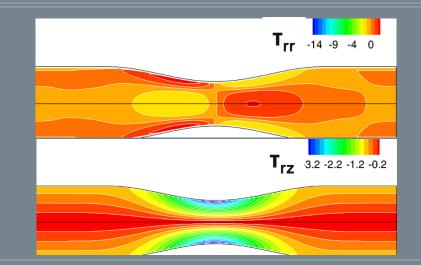
Heart Valve

 Study the hemodynamics of healthy & pathological native & prosthetic leaflets at physiological flow conditions.



Viscoelastic hemodynamics in stenotic microvessels

• Examine the hemodynamics in stenotic micro-vessels by using constitutive models for the blood that account or RBC populations and viscoelasticity.





- Tsamopoulos, J., Dimakopoulos, Y Chatzidai N., Karapetsas, G. and Pavlidis M., "Steady bubble rise and deformation in Newtonian and viscoplastic fluids and conditions for bubble entrapment" J. Fluid Mech., 601, 123–164 (2008).
- Chatzidai, N. Giannousakis, A. Dimakopoulos, Y. and Tsamopoulos, J. "On the elliptic mesh generation in domains containing multiple inclusions and undergoing large deformations", J. Comp. Phys. 228 1980–2011 (2009).
- Dimakopoulos, Y. & Tsamopoulos, J., "On the transient coating of a straight tube with a viscoelastic material", J. Non Newt. Fluid Mech., 159, 95-114 (2009).
- Papaioannou, J., Karapetsas, G., Dimakopoulos Y. and Tsamopoulos, J. "Injection of a viscoplastic material inside a tube or between parallel disks: conditions for wall detachment of the advancing front J. Rheol. 53(5), 1155-1191 (2009).
- Pavlidis, M., Dimakopoulos, Y. and Tsamopoulos, J. 'Fully developed flow of a viscoelastic film down a vertical cylindrical or planar wall", Rheol. Acta., 48(9), 1031-1048, (2009).
- Karapetsas, G. and Tsamopoulos, J. "On the stick-slip flow from slit and cylindrical dies of a Phan-Tien and Tanner fluid model: I. Steady state", Phys. Fluids., 21, 123101 (2009) (18 pages).
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- Dimakopoulos, Y., "An efficient parallel fully implicit algorithm for the simulation of transient free surface flows of multimode viscoelastic liquids", J. Non-Newtonian Fluid Mech., 165 (7-8), 409-424 (2010).
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- Dimakopoulos, Y., Bogaerds, A., Anderson, P., Hulsen, M., Baaijens, F.P.T., "Direct numerical simulation of a 2D idealized aortic heart valve at physiological flow rates", Comp. Meth. Biomech. and Biomed. Engrg, 15 (11), 1157-1179 (2012).
- Tseropoulos, G., Dimakopoulos, Y., Tsamopoulos, J., Lyberatos, G. "On the flow characteristics of the conical Minoan pipes used in water supply systems, via computational fluid dynamics simulations", J. Archeol. Sci. 40, 2057-2068 (2013).
- Karapetsas, G. and Tsamopoulos, J. "On the stick-slip flow from slit and cylindrical dies of a Phan-Tien and Tanner fluid model: II. Linear stability analysis to two- and three-dimensional disturbances", Phys. Fluids, 25, 093105 (2013),



- "Critical forming technologies for producing CMOS circuits with dimension <100nm in industrial scale", GSRT/PENED, 160 k€, share of our lab was 52 K€, for 3 years, start 2005.
- "Multi-scale modelling of interfacial phenomena in acrylic adhesives undergoing deformation, Proposal acronym: MODIFY", EU, 3100 k€, share of our lab was 300 k€, for 3 years, start 2009.
- "Film rupture of nanostructured liquids in processing of composite materials" GSRT/Heraklitos program, 45 k€, for 3 years, start 2010.
- Complex Visco-elastic and Visco-plastic Materials: From Microscopic Structure and Dynamics to Macroscopic Flow" COVISCO, GSRT/Thales program, 600 k€, share of our lab was 70 k€, for 45 months, start 2012.
- "Thin film flows of complex fluids in microfluidic applications", FilCoMicrA, GSRT/Excellence program, Grant Number: 1918, 300 k€, for 3 years, start 2012.







Dr. Dionisis Photeinos Dr. Phuc-Khan Nguyen Bubble Dynamics Thin Film Flows

Nguyen Dr. Micha

Dr. Michalis Pavlidis Thin Film Flows & Bubble Dynamics



Dr. Giorgos KarapetsasYannis Papaioannou Interfacial Wetting and instabilities Spreading Senior Researchers Post Doctoral Researchers

> PhD Candidates Graduate Students (5 in total)

Undergraduate Students (7 in total)



Dionisis Pettas Interfacial instabilities



stasis Giannousak Complex Flows



Sophia Tsouka Polymer migration phenomena



Yannis Vasilopoulos Multiphase Flows



Dimitris Fraggedakis Multiphase Flows

Simulation of complex & biological flows