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**PERSONAL**

Date of birth: January 4, 1966

Marital status: Married (with Vasiliki Mavrozoumi; have 1 son, George)

Citizenship: Greek

Languages: English, Greek, some German

Leisure activities: Literature and poetry reading, listening to radio, playing soccer

**ACADEMIC INTERESTS**

* Physical Chemistry, Chemical Engineering Thermodynamics, Statistical Thermodynamics, Non-equilibrium Thermodynamics
* Statistical Mechanics, Molecular Simulations
* Dynamics and Rheology of micro-structured fluids
* Finite-Element and Spectral-Element Numerical Methods

**RESEARCH INTERESTS**

* Modeling and simulation of polymers and of soft nanostructured polymeric materials at multiple time and length scales (atomistic, mesoscopic, macroscopic)
* Multiscale modeling of chain dynamics and rheology (viscoelasticity) in polymers as a function of the molecular architecture of the chains (linear, branched, rings)
* Modeling polymers at interfaces (adhesion, self-assembly, dynamics in confined geometries)
* Thermodynamics of complex fluids under non-equilibrium conditions
* Constitutive modeling of polymer viscoelasticity
* Molecular modelling and simulation of the phase state of atmospheric organic aerosol particles, and prediction of their physicochemical properties
* Quantum Field Theory

**EDUCATION**

Ph.D. in Chemical Engineering

University of Delaware, Newark, Delaware, April 1994

• *GPA*: 4.0/4.0

• *Dissertation*: "Surface effects on the conformation and rheology of polymer solutions"

• *Advisor*: Prof. A.N. Beris

• *Minor*: Mathematics and Physics (GPA: 4.0/4.0)

Diploma in Chemical Engineering

National Technical University (NTU), Athens, Greece, July 1988

• *GPA*: 9.24/10.00 (top 1%)

• *Diploma thesis*: "Regional energy planning in the islands of the Cyclades complex"

• *Advisor*: Prof. M. Koukios

**PROFESSIONAL EXPERIENCE**

Dozent-Lecturer (September 2016- today)

Department of Mechanical and Process Engineering (with Prof. S.E. Pratsinis), Particle Technology Laboratory, ETH Zürich, Switzerland

Guest Professor (September 2014- September 2016)

Department of Mechanical and Process Engineering (with Prof. S.E. Pratsinis), Particle Technology Laboratory, ETH Zürich, Switzerland

Guest Professor (September 2013- August 2014)

Department of Materials Science (with Prof. Hans Christian Öttnger), Institute of Polymers, ETH Zürich, Switzerland

Professor (July 2011-today)

Department of Chemical Engineering, University of Patras, Patras, Greece

Associate Professor (July 2003-July 2011)

Department of Chemical Engineering, University of Patras, Patras, Greece

Researcher B’ (November 2001-July 2003)

Institute of Chemical Engineering and High-Temperature Chemical Processes, ICE/HT-FORTH, Patras, Greece

Researcher C’ (October 1997-October 2001)

Institute of Chemical Engineering and High-Temperature Chemical Processes, FORTH-ICE/HT, Patras, Greece

Post-Doctoral Research Assistant (January 1996-October 1997)

Institute of Chemical Engineering and High-Temperature Chemical Processes and Department of Chemical Engineering, University of Patras, Patras, Greece

Military Service (May 1994-December 1995)

War Material Corps, Didymoteicho, Evros, and Army Chemistry Labs, Piraeus, Greece

Ph.D. Research Assistant (September 1989-April 1994)

Department of Chemical Engineering, University of Delaware, USA

**OTHER PROFESSIONAL ACTIVITIES**

Visiting Scientist

* Institute of Polymers, Department of Materials, ETH-Zürich, Switzerland (January-February 2013, June-July 2012, February 2006, February 2002, February 2000, with Prof. Hans Christian Öttinger)
* Technical University of Denmark (DTU), Lyngby, Denmark (June-July 2010, with Prof. George Kontogeorgis)
* Norwegian University of Science and Technology (NTNU), Trondheim, Norway (February 2010, with Prof. Zhiliang Zhang)
* Department of Applied Physics, University of Tokyo, Japan (June-July 2005, with Prof. Masao Doi)
* Dow Chemical Company, Midland, USA (December 2000, with Dr. Joey Storer)
* University of Delaware, Department of Chemical Engineering, Newark, DE, USA (August 1999, with Prof. Antony Beris)

Collaborating Faculty Member

* Inter-Departmental Programme of Graduate Studies in “Polymer Science and Technology”, University of Patras (1999-today)

- Department of Materials Science, University of Patras (2000-2002)

National Delegate

* In the Working Party on Thermodynamics and Transport Properties (WP-TTP), one of the seventeen WPs of the European Federation of Chemical Engineering (EFCE)

**HONORS**

* Associate Editor, *Frontiers in Physics*, Open Access Scholarly Publishers Association (since 2018)
* On the International Advisory Board of the Journal: *Macromolecular Theory and Simulation*, Wiley-VCH, Germany, since 2005
* The Allan P. Colburn Prize in Engineering and Mathematical Sciences, for the PhD thesis dissertation titled: “Surface Effects on the Structure and the Rheology of Dilute Polymer Solutions”, University of Delaware, 1993-1994
* University of Delaware Competitive Fellowship, 1991-1992
* Thomaidis Excellence Award for graduating first in class of 1988, NTUA
* Economou Excellence Award for graduating first in class of 1988, NTUA
* Technical Chamber of Greece Excellence Award for graduating first in class of 1988, NTUA
* Outstanding Undergraduate Student Excellence Awards, annually 1983-1988, NTUA

**PROFESSIONAL AFFILIATIONS**

* Member, American Institute of Chemical Engineers (AIChE)
* Member, American Physical Society (APS)
* Member, Society of Rheology (SOR)
* Member, Polymer Processing Society (PPS)
* Member, Technical Chamber of Greece (TEE)
* Secretary, Hellenic Society of Rheology (HSR)

**ADMINISTRATIVE POSITIONS**

* Secretary-Treasurer, Hellenic Society of Rhoelogy (HSR), September 206-to date
* President of the Hellenic Society of Rheology (HSR), September 2004-September 2006
* Director, Inter-department Programme of Graduate Studies on “Polymer Science and Technology”, University of Patras, 2003-2013

## RESEARCH ACTIVITIES

### ***1) Multi-scale modeling of soft nanostructured materials based on polymer adhesives***

Soft nanostructured materials based on polymers overwhelm the modern adhesives industry due to a spectrum of unique properties such as excellent control on glass transition temperature, low plateau modulus, competitive cost, superior stability, and greater resistance to oxidation (because of their saturated backbone) compared to rubber-based analogues. Within these materials, interfaces pose specific challenges, since they are usually diffuse and can transfer stress through chain entanglements. For example, acrylic PSAs are based on complex formulations employing random copolymers of a long-chain acrylic (e.g., n-butyl acrylate, BA) characterized by a low glass transition temperature (Tg) with a short side-chain acrylic (such as methyl acrylate) to adjust Tg and acrylic acid (AA) to improve adhesion and optimise elongational properties. When they are prepared by emulsion polymerisation in water, they result from the drying and coalescence of separate latex particles so that the memory of the *original interface* is retained. In applications involving a contact between the soft polymer and a hard substrate, *interfacial bonding* also constitutes a fundamental problem, since it is at the root of the mechanisms governing failure upon deformation. In our lab, we try to get a fundamental understanding of the role of all these interfaces in the performance of acrylic adhesives by developing sophisticated hierarchical models addressing:

* the mechanism(s) of stress transfer at internal interfaces between soft latex particles containing polymers with different topologies; this needs to be addressed at different scales from the molecular to entanglement network level
* the mechanism of stress transfer at hard-soft interfaces between the substrate and the soft adhesive, as a function of chemical composition of the PSA formulation and the chemistry of the substrate
* the effect of the presence of multiple internal interfaces on the macroscopic deformation behaviour of the adhesive
* how cavitation and the development of the fibrillar structure in the final adhesive product are affected by changes in the properties of the initial formulation
* the respective role played by the polymer rheology
* the correct type of boundary conditions (b.c.’s) at the polymer/substrate interface; this needs to be derived from non-equilibrium statistical mechanics
* a more representative constitutive law for the finite isotropic and anisotropic elastic behaviour of these materials

***2) Polymer membranes based on carbon nanotubes***

Polymeric materials such as polycarbonate (PC), polystyrene (PS) and PMMA incorporating aligned carbon nanotubes show great potential for use as novel membrane systems. This happens because their nanoscale structures mimics the selective transport and extraordinarily fast flow possible in biological cellular channels with a wide range of potential applications. Indeed, it has been shown that membranes based on polymer encapsulation of aligned carbon nanotube (CNT) arrays exhibit unusual enhancements in transport rates and non-Knudsen selectivities for gas mixtures and water, mainly due to the almost frictionless interface at the carbon-nanotube walls. Thus, water flow rates through them are measured to be four to five orders of magnitude faster than conventional fluid flow would predict through pores of 7 nm diameter. CNTs are also imbedded in polymeric matrices in order just to achieve simply structural reinforcement (improvement of the mechanical properties of the resulting nanocomposites). Although a considerable amount of research has been devoted in the literature to understand the factors that govern mechanical strength and the barrier properties of CNT/polymer nanocomposites, a comprehensive understanding is still lacking. We try to fill this gap by pursuing a computational materials design approach which utilizes state-of-the-art multiscale modelling:

* It starts from the atomistic level and goes all the way up to predicting deformation and failure phenomena by establishing links between the various levels of description, thereby addressing different length and time scales. In this hierarchy, each level of modeling receives input from more fundamental levels and provides input to more coarse-grained ones.
* It employs state-of-the-art computational methods at each level to address the relevant phenomena such as multiple time step and/or accelerated dynamics MD schemes and novel kinetic MC algorithms.

Our goal is predict the transport properties (solubility, diffusion, and pressure-driven flow rates) of small fluid molecules first through a CNT and then through the CNT-polymer membrane, for selected polymer chemistries and small penetrant molecules.

***3) Polymer nanocomposites based on graphene***

Incorporating nanosized particles in a polymer matrix can lead to new materials with significantly improved mechanical, electrical, optical, and thermal properties. This explains the large body of theoretical, modeling and experimental work accumulated recently, in an effort to address the complex interplay between molecular-level parameters and mechanisms in polymer nanocomposites (PNCs), and macroscopically-manifested properties. But there exist many issues still not well understood such as: a) how one can control nanoparticle (NP) dispersion and what are the molecular or thermodynamic parameters controlling the phase behavior of PNCs?; b) how does the presence of NPs alter the conformational and relaxation properties of the polymer?; c) how are the linear and non-linear viscoelastic properties of the pure polymer matrix changed as a function of the volume fraction and size of the added NPs; d) what is the respective role of the size of polymer chains relative to the NP diameter?; e) what are the relevant contributions of enthalpic and entropic effects?; f) how does chain end-grafting onto a spherical NP alter nanoparticle dispersion, thus also the mechanical and rheological properties of the resulting nanocomposite?

We try to address many of these questions through direct simulation efforts preferably through the design of multi-scale methodologies but also through the development of constitutive models based on a minimal set of state variables representative of the system under study.

Properties to be predicted here include: a) For the bulk polymer matrix: the density, characteristic ratio, static structure factor, distribution of torsion angles, relaxation modulus, entanglement length, viscosity, storage and loss moduli, and free volume, all as a function of temperature. b) For the PNC: structure, conformation, volumetric behavior, work of adhesion, interfacial shear strength, elastic moduli, and rheology in linear and non-linear regimes, all as a function of temperature, applied deformation or shear rate, and nanoparticle volume fraction.

##### *4) Constitutive equations for polymer melts guided by principles of nonequilibrium thermodynamics*

Based on principles of nonequilibrium thermodynamics, we derive generalized differential constitutive equations for polymer melts which incorporate terms that account for anisotropic hydrodynamic drag in the form suggested by Giesekus, finite chain extensibility with non-linear molecular stretching, non-affine deformation, and variation of the longest chain relaxation time with chain conformation. In the new equations, the expression for the Helmholtz free energy of deformation is defined such that the entropy remains bounded even at high deformation rates, as it should from a physical point of view. Key elements in the new constitutive models are the functions describing the dependence of the nonequilibrum free energy and relaxation matrix on the conformation tensor. Restrictions on the parameters entering these two functions are obtained by analyzing the thermodynamic admissibility of the model. With suitable choices of these two functions, the new equations reduce to a number of well-known viscoelastic models. However, they are more general in the sense that they permit incorporating into a single constitutive differential equation more accurate expressions for the description of chain elasticity and relaxation. The new equations are used to describe (fit) rheological data provided either by experimental measurements on industrial samples or obtained through Non-Equilibrium Molecular Dynamics (NEMD) simulations in shear and planar elongation.

***5) Topological and dynamical mapping of atomistic simulation results onto the tube model of the reptation theory for the dynamics of entangled polymers***

A number of approaches have been reported in the last years capable of identifying topological constraints and generating ensembles of primitive paths in entangled, multi-chain polymeric systems. In addition to providing predictions for the static (statistical) properties of the underlying entanglement network, these approaches have opened up the way to interfacing atomistic simulation data with reptation, admittedly the most successful phenomenological theory of polymer dynamics for entangled systems. We are developing such a link between atomistic molecular dynamics simulation results and reptation theory by geometrically constructing the effective tube around each primitive chain and then documenting chain motion in terms of a curvilinear diffusion inside the effective tube around the coarse-grained chain contour. The outcome of such a topological and dynamical mapping is the computation of observables quantifying reptation in entangled polymers. A typical example is the function *ψ*(*s,t*), namely the probability that a segment *s* of the primitive chain remains inside the initial tube after time *t*. We try to utilize this information in order to bring together three different approaches to polymer dynamics (in addition to acquiring reliable experimental data): atomistic simulations, mesoscopic entanglement networks, and tube models. By consistently mapping the results of accurate computer models of polymer structure and dynamics onto theoretical treatments based on phenomenological concepts (that sometimes defy precise definition) on some well-defined model systems, we hope to get a deeper understanding of the predominant relaxation mechanisms in entangled polymers, and thus succeed in our effort to encode this information in the form of suitable (more accurate) constitutive equations.

***6) Multiscale modeling and simulation of polymer-based materials for use in microelectronics***

Charge transfer in organic semiconducting polymers (which are often characterized by a π-conjugated backbone) is sensitive to conformational disorder along the main chain backbone and to chemical defects in the bulk of the material. Thus, despite intense basic research in the field for more than a decade, only few polymer-based devices for electronic transport have been realized up to now. In general, charge mobility in polymer semiconductors is strongly dependent on morphology at the molecular level but also at the level of entire chains (e.g., the chain end-to-end distance). At even larger scales, polymer semiconductors consist usually of crystalline domains separated by amorphous regions. This happens because molecules in low molecular-weight (MW) films are able to form well-ordered crystals more easily than molecules in high-MW films. Thus, to understand charge transport one needs to understand first self-assembly at the nano-scale where crystalline and amorphous domains co-exist but also close to the electrodes where chains are practically sandwiched between two metallic plates. Depending on the environmental conditions, the disordered polymer layer is also doped with ions, which further affect charge transport through the material. The motion of charge carriers in these systems, particularly between different chains, is sensitive to local ordering, and although the link between high ordering and charge mobility is well established, quite often the need to optimize chain packing comes up with additional challenges. For example, the addition of alkyl side chains (which helps improve solubility and reduce the melting temperature increases the distance between polymer chains) leads to considerably reduced charge transfer along the chain direction. Also, usually, and despite this higher local ordering in low-MW samples, higher charge mobility are observed in films of high-MW polymer semiconductors.This can be explained by the fact that longer polymer chains are able to form bridges between different crystalline domains. Using as model systems conjugated polymers that are known to form morphology at the nano-scale (e.g., two-dimensional sheets) such as P3HT, PQT, and PBTTT, in our team we develop multi-scale modelling tools addressing:

* microstructure and morphology development at the nanoscale due to self-assembly, the dominant assembling mechanisms, and the resulting supramolecular arrangement of the formed two-dimensional foils or layers
* structural properties in the crystalline and amorphous regions (such as inter-ring and ring-tail torsions, long-range correlations between the orientations of thiophene rings and their temperature dependence, radial distribution functions, interchain spacing), also between the nano-domains and how they affect the charge-transfer behavior
* the effect of regioregularity (stereo-regular versus random-regular) on the self-assembly properties of these systems and eventually on their charge-transfer behavior
* the presence of defects in the crystal structure as a function of temperature through large scale classical molecular dynamics simulations
* intra- versus inter-chain contributions to charge mobility and their dependence on torsional defects and the inter-chain (lamellae) spacing

***7) Atomistic simulation of the dynamics of ring polymers***

Ring polymers is a special case of chain molecules since they have no ends; as a result they are topologically different than linear counterparts (and/or long chain branched polymers) for which their viscoelasticity is typically described by the reptation theory and variants of the tube model. In addition, it is experimentally believed that the presence of even a small percentage of linear polymers in the ring has a profound effect on their dynamics, causing a significant reduction in their relaxation, thus also on diffusion and viscosity. In an effort to understand the unique rheological properties of ring polymers, we have embarked on a new project involving three steps:

# generation and detailed atomistic molecular dynamics simulations of model polyethylene and polyethylene oxide ring melts (both short and long chain length)

# comparison of simulation results for the chain diffusivity, zero shear rate viscosity, and neutron scattering pattern against similar data from direct experimental measurements

# extension to blends of linear and ring PEO systems – dependence of dynamic properties on blend composition and chain length

# analysis of the simulation results and mapping onto recent theories for entangled rings

# development of methodologies for the topological analysis of ring polymers

# extension to beyond equilibrium conditions by use of non-equilibrium molecular dynamics (NEMD) simulations, in an effort to capture the flow behavior of polymer ring melts which at present is totally unknown

***8)*** ***Hierarchical simulation of microcrystalline PECVD silicon film growth and structure***

Plasma enhanced chemical vapor deposition (PECVD) is a popular technique for growing Si films. The high growth rates obtained by exploiting the presence of reactive radicals in the gas phase render this technique of industrial interest, since it allows for the fast deposition of thin films even at moderately low temperatures, since no thermal cracking is required. By tuning the growth parameters, PECVD can be used to grow epitaxial, amorphous, and micro- (μc) or nanocrystalline (nc) films. Being promising for the production of solar cells with a good efficiency/cost ratio, nc-Si films have attracted recently wide attention. Our goal here is to design and implement hierarchical simulation methodologies for the study of PECVD of silicon films, the emphasis placed on the elucidation of the microscopic mechanisms as well as the interplay between atomic level and macroscopic design parameters associated with the development of nano- or micro-scale crystalline regions in the grown layer. The ultimate goal is to use multi-scale modeling as a design tool for tackling the issue of local crystallization depending on the environment, thus also of the growth parameters. Our simulation approach is based on the design of a very efficient, large-scale kinetic Monte Carlo (kMC) algorithm capable of generating samples of representative Si films based on a validated chemistry model. In a second step, the generated film is subjected to an atomistic simulation study restoring the molecular details lost or ignored in the kMC model and tuning the local structure i.e. the important morphological details associated with the presence of crystalline and amorphous regions (and the intervening interfacial domains) in the grown film. The kMC method is based on a carefully chosen set of reacting or active radicals (species) in the gas phase impinging the film and a detailed set of surface reactions. For a three-dimensional Si(001)-(2x1):H crystalline lattice, our kMC method allows us to study several seconds of film growth, resulting in thicknesses in the order of tenths of nanometers. The kMC method has been validated by carrying out computational experiments over a wide range of dilution ratios and by comparing the numerical results for the growth rate and roughness with the corresponding experimental data; very good agreement is observed in most cases. In a final step, the 3-d structures generated with kMC are used as input in large-scale MD simulations for times up to several microseconds to allow the system further relax towards the preferred morphological state at the conditions of interest. This allows us to obtain predictions for other industrially relevant quantities and observables (e.g. hydrogen content and crystallinity which are experimentally accessible by FTIR and Raman spectroscopy), thus opening the way to fully understanding the underlying complex molecular mechanisms responsible for the growth of micro- or nanocrystalline films.

## PARTICIPATION IN RESEARCH AND DEVELOPMENT PROJECTS

NATIONAL PROJECTS

*PROSMAK [1]:*

* GSRT PENED 2001 project titled: *The role of grafted macromolecules to the stability of nanoparticles (applications to the technology of paintings)*
* Code: 01ED587
* partners: FORTH-ICE/HT (coordinator), University of Patras, FORTH-IESL, INTERCHEM-HELLAS
* Total budget: 220 kEuro
* Contribution to the Lab: 50 kEuro
* Duration: 2002-2005
* Project Coordinator: V.G. Mavrantzas

*ESOPO [2]*

* GSRT PENED 2001 project titled: *Study of the effects of mechanical stress and temperature in the extrusion of reinforced polyethylene pipes*
* Code: 01ED136
* Partners: FORTH-ICE/HT (coordinator), University of Patras, Petzetakis SA
* Total budget: 193.7 kEuro
* Contribution to the Lab: 46 kEuro
* Duration: 2002-2005
* Project Coordinator: V. Gregoriou

*AKMON 2004 [3]*

* GSRT project titled: *Design and characterization of heterogeneous materials for applications in the technologies of energy and environment*
* Partners: FORTH-ICE/HT (coordinator), University of Patras
* Total budget: 481 kEuro
* Contribution to the Lab: 106 kEuro
* Duration: 2004-2007
* Project coordinator: V. Burganos

*Karatheodori 2004 [4]*

* University of Patras project titled: *Prediction of the structural and interfacial properties of aqueous solutions of n-alkyl poly(oxy ethyl ethers) from molecular simulations*
* Partners: University of Patras
* Total budget: 40.5 kEURO
* Contribution to the Lab: 23.5 kEuro
* Duration: 2004-2007
* Project coordinator: V.G. Mavrantzas

*Pythagoras II 2004 [5]*

* Ministry of Education of Greece project titled: *New numerical techniques for the computation of flows of viscoelastic materials under conditions of industrial applications*
* Partners: University of Patras
* Total budget: 50 kEuro
* Contribution to the Lab: 25 kEuro
* Duration: 2005-2007
* Project coordinator: J. Tsamopoulos

*HERACLITUS [6]*

* National project titled: *Molecular mechanisms governing slip phenomena during the flow of polymeric melts past solid substrates*
* Partners: UPatras
* Total National contribution: 45 kEuro
* National contribution to the Lab: 45 kEuro
* Duration: 2010-2013
* Project coordinator: V.G. Mavrantzas

*MEKKA [7]*

* National project (synergasia) titled: *Development of carbon nanotube based polymeric membranes for industrial wastewater treatment and water reuse*
* Contract No: 620-11/11/2009
* Partners: FORTH-ICE/HT, UPatras, INTERCHEM
* Total National Contribution: 425 kEuro
* EC contribution to the Lab: 80 kEuro
* Duration: 2011-2013
* Project coordinator: V.G. Mavrantzas

*THALES [8]*

* National project (Thales) titled: *Graphene and its nanocomposites: Production, properties and applications*
* Partners: FORTH-ICE/HT
* Total National Contribution: 400 kEuro
* Contribution to the Lab: 30 kEuro
* Duration: 2012-2015
* Project coordinator: C. Galiotis

*ARISTEIA 2011 [9]*

* National project (Aristeia 2011) titled: *General method for the simulation of self-organization in nanostructured polymeric systems*
* Partners: Univ. of Patras
* Total National Contribution: 300 kEuro
* Contribution to the Lab: 300 kEuro
* Duration: 2012-2015
* Project coordinator: V.G. Mavrantzas

*RINGS [10]*

* National research project (GSRT, Support of reserachers with emphasis to new researchers) titled: *Conformational and transport properties of solutions of synthetic and biological cyclic polymers: theory and atomistic simulation (RING-Solutions)*
* Contract No: 5004866
* Partners: FORTH-ICE/HT
* Total contribution: 59,85 kEuro
* EC contribution to the Lab in Patras: 59.85 kEuro
* Duration: 2018-2019
* Project coordinator: Vlasis Mavrantzas

*PNC\_RHEO [11]*

* National research project (GSRT, Support of researchers with emphasis to young researchers) titled: *Study of the rheology of polymer nanocomposite melts by combining molecular simulations and rheological constitutive modelling (PNC\_Rheo)*
* Contract No: to be given
* Partners: UPatras
* Total contribution: 41.5 kEuro
* EC contribution to the Lab in Patras: 41.5 kEuro
* Duration: 2019-2020
* Project coordinator: Vlasis Mavrantzas

*RINGS [12]*

* National research project (FORTH Synergy Grant) titled: *Shear and extensional rheology of entangled ring polymer melts (RINGS)*
* Contract No: to be given
* Partners: FORTH-IESL, FORTH-ICE/HT
* Total contribution: 80 kEuro
* EC contribution to the Lab in Patras: 25 kEuro
* Duration: 2019-2021
* Project coordinator: Dimitris Vlassopoulos

EUROPEAN (EC) PROJECTS

*GeMColloidS [1]*

* EC research project (MARIE-CURIE Host Development Fellowship) titled: *Generic Methodologies in Colloids and Suspensions*
* Contract No: HPMD-CT-2000-00054
* Partners: FORTH-ICE/HT
* Total EC contribution: 228 kEuro
* EC contribution to the Lab: 228 kEuro
* Duration: 2001-2004
* Project coordinator: V.G. Mavrantzas

*PMILS [2]*

* EC Growth research project titled: *Polymer Modeling at Integrated Length/Time Scales*
* Contract No: G5RD-CT-2002-00720
* Partners: UPM (Coordinator), FORTH-ICE/HT, Borealis, Rhodia, NKT, DTU, Imperial College, CPERI, Namur, Ip-Sol
* Total EC contribution: 2,689 kEuro
* EC contribution to the Lab: 423.1 kEuro
* Duration: 2002-2005
* Project Coordinator: Manolo Laso
* Research leader from FORTH-ICE/HT: V.G. Mavrantzas

*MODIFY [3]*

* EC (FP7-NMP-2008-SMALL-2) project titled: *Multi-scale modeling of interfacial phenomena in acrylic adhesives undergoing deformation*
* Contract No: 228320
* Partners: Univ. of Patras (coordinator), ESPCI, CNRS, UCL, ETH-Z, DOW, LBI
* Total EC contribution: 2,863 kEuro
* EC contribution to the Lab: 402.3 kEuro
* Duration: 2009-2012
* Project coordinator: V.G. Mavrantzas

*PEPPER [4]*

* EC (FP7-ENERGY-2009-TREN-2) project titled: *Demonstration of high performance processes and equipments for thin film silicon photovoltaic modules produced with lower environmental impact and reduced cost and material use*
* Contract No: 249782
* Partners: OS (coordinator), IMT, UPatras, UoN, ETF, HSPH, Linde
* Total EC contribution: 9,380 kEuro
* EC contribution to the Lab: 60 kEuro
* Duration: 2010-2013
* Project coordinator: Tobias Roschek
* Project leader from the University of Patras: D. Mataras

*BioNexGen [5]*

* EC (FP7-NMP-2009-SMALL-3) project titled: *Development of the next generation membrane bioreactor system*
* Contract No: 246039
* Partners: HSKA (Coordinator), CNR-ITM, UON, FORTH, SEZ, MN, IZTECH, ABU, CMRDI, CBS, NTX
* Total EC contribution: 3,420 kEuro
* EC contribution to the Lab: 60 kEuro
* Duration: 2010-2013
* Project coordinator: Jan Hoinkis
* Project leader from FORTH-ICE/HT: G. Vogiatzis

*MMM@HPC [6]*

* EC (FP7-INFRA-2010-1.2.2) project titled: *Multiscale materials modeling on high performance computing*
* Partners: KIT (Coordinator),CSC-IT, UPatras, UMons, CEA Grenoble, CINECA Bologna, Li-Tec Battery, BASF, Nokia, Sony
* Total EC contribution: 2,800 kEuro
* EC contribution to the Lab: 214 kEuro
* Duration: 2011-2013
* Project coordinator: Wolfgang Wenzel
* Project leader from the University of Patras: V.G. Mavrantzas

*BioSmartTrainee [7]*

* EC research project (H2020-MSCA-ITN-2014) titled: *Training in Bio-Inspired Design of Smart Adhesive Materials (BioSmartTrainee)*
* Contract No: DYNACOP
* Partners: LIFP-Dresden (coordinator), MPI-P, WU, ESPCI, BASF, Cambridge Univ., TUE, UPatras, AkzoNobel, URGO
* Total EC contribution: ~ 2,822 kEuro
* EC contribution to the Lab: 221 kEuro
* Duration: 2015-2018
* Project coordinator: Alla Synytska (LIFP-Dresden)
* Project leader from UPatras: V.G. Mavrantzas

*FORCE [8]*

* EC research project (H2020-NMBP-2016-2017) titled: *Formulations and Computational Engineering (FORCE)*
* Contract No: FORCE
* Partners: Dow, Unilever UK, IBM-Zurich, Fraunhofer IWM/ITWM, Enthought Ltd., EnginSoft Spa, Granta Design Ltd., UPatras, Megara Resins S.A., ETH-Z
* Total EC contribution: ~ 5,417 kEuro
* EC contribution to the Lab in Patras: 294.1 kEuro
* EC contribution to the Lab in Zurich: 478.5 kEuro
* Duration: 2016-2020
* Project coordinator: Adham Hashibon (Fraunhofer IWM/ITWM)
* Project leader from UPatras: V.G. Mavrantzas

INDUSTRIAL PROJECTS

#### Dow Chemicals Industrial Project Ι [1]

* Industrial research project with Dow Benelux B.V. titled: *Multi-scale simulation of polyethylene melt rheological and processing properties*
* Contract No: Research contract with the Dow Chemical Company (USA and The Netherlands)
* Partners: FORTH-ICE/HT (coordinator), Dow Benelux (Netherlands)
* Total budget: 86.4 kUSD
* Contribution to the Lab: 86.4 kUSD
* Duration: 2002-2005
* Project coordinator: V.G. Mavrantzas

#### DOW Chemicals Industrial projectII [2]

* Industrial research project with Dow Benelux B.V. titled: *Multi-scale simulation of polyethylene melt rheology and processing properties*
* Contract No: Research contract with Dow Chemical Company (USA)
* Partners: FORTH-ICE/HT (coordinator), Dow Benelux (Netherlands), Dow Chemical Company (USA)
* Total budget: 75 kEuro
* Contribution to the Lab: 75 kEuro
* Duration: 2006-2008
* Project coordinator: V.G. Mavrantzas

*Limmat [3]*

* Limmat Foundation donation project (MuSiComPS) titled: *Multiscale Simulations of Complex Polymer Systems (MuSiComPS)*
* Contract No: MuSiComPS
* Partners: NTUA, UPatras
* Total Limmat Foundation contribution: ~1000 kEuro
* Contribution to the Lab: 320 kEuro
* Duration: 2015-2020
* Project coordinator: D.N. Theodorou
* Project leaders from UPatras: V.G. Mavrantzas, J. Tsamopoulos

OTHER PROJECTS

*NATO CRG 1998 [1]*

* NATO collaborative research grant titled: *From the Rouse to the Entangled Polymer Melt Regime*
* Contract No: CRG.CRG.973023
* Partners: FORH-ICE/HT, Univ. of Delaware (USA)
* Budget: 216 kBEF
* Contribution to the Lab: 216 kBEF
* Duration: 1998-2000
* Project Coordinator: V.G. Mavrantzas

*NATO CRG 2001 [2]*

* NATO collaborative linkage grant titled: *Structure and Dynamics in Crystalline Polymers: Vibrational Spectroscopy and Molecular Simulation*
* Contract No: CRG.CRG.973023
* Partners: FORH-ICE/HT, MIT, University of Jerusalem
* Total budget: 8,000 USD
* Contribution to the Lab: 8,000 USD
* Duration: 2001-2003
* Project Coordinator: V.G. Mavrantzas

**PUBLICATIONS IN REFEREED JOURNALS (\* denotes corresponding author)**

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*Chapter 7*: Coarse-graining

*Chapter 8*: Entanglement network-based simulations of deformation and flow

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71. F.D. Tsourtou, **V.G. Mavrantzas**, “Atomistic Monte Carlo and Molecular Dynamics simulation of nanostructured semiconducting polymers and polypeptides”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
72. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, “Comparison of the conformational and dynamic properties between ring and linear polyethylene oxide melts in the crossover region from unentangled to entangled through molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
73. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, “Study of water molecule mobility in carbon nanotubes embedded in a PMMA matrix”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
74. D. Mallios, D.G. Tsalikis, **V.G. Mavrantzas**, “Self-assembly of amphiphile peptides into nanostructures through detailed molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
75. C.Κ. Georgantopoulos, I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, “Development of state-of-the-art constitutive rheological models for entangled polymeric fluids using principles of nonequilibrium thermodynamics”,*11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
76. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, “On the effect of end-functionalized groups on the dynamics of polymer melt nanocomposites through molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
77. A. Spyrogianni, K.K. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Brownian dynamics simulation of the settling rate of fractal-like nanoparticle agglomerates”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**

**PRESENTATIONS** (speaker underlined)

1. **V.G. Mavrantzas**, A.N.Beris, “Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions”, *March Meeting of the American Physical Society*, Cincinnati, March 18-22, **1991**.
2. **V.G. Mavrantzas**,A.N. Beris, “Theoretical study of the effects of solid/fluid interface on the rheology of polymer solutions”, *"Symposium on Interfacial Phenomena in Viscoelastic Flows*" organized by the Fluid Mechanics Committee of the Applied Mechanics Division of ASME, Columbus, June 16-19, **1991**.
3. **V.G. Mavrantzas**, A.N. Beris, “Theoretical Study of wall effects on the rheology of dilute polymer solutions”, *Society of Rheology Meeting*, Rochester, October 20-24, **1991**.
4. **V.G. Mavrantzas**, A.N. Beris, “Modeling and simulation of the dilute polymer solution flow behavior next to solid surfaces and interfaces”, *National Meeting of the American Chemical Society*, San Francisco, April 5-10, **1992**.
5. **V.G. Mavrantzas**, A.N. Beris, “Interfacial phenomena in the rheology of dilute polymer solutions”, *AIChE Annual Meeting*, Miami Beach, November 1-6, **1992**.
6. A.N. Beris, **V.G.** **Mavrantzas**, “Non-local effects in polymer rheology: Polymer-surface interactions”, *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
7. **V.G. Mavrantzas**, A.N. Beris, “Stress-induced polymer migration phenomena in simple viscometric flows”, *Society of Rheology Meeting*, Boston, October 17-21, **1993**.
8. **V.G. Mavrantzas**, A.N. Beris, “Rheology of dilute polymer solutions in the adjacency of a solid surface”, *AIChE Annual Meeting*, Saint Lewis, November 7-11, **1993**.
9. **V.G. Mavrantzas**, A.N. Beris, “Polymer migration in simple viscometric flows”, *AIChE Annual Meeting*, Saint Lewis, November 7-11, **1993**.
10. **V.G. Mavrantzas**, D.N. Theodorou, “From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques’’, *EPF Annual Meeting*, Aghia Pelaghia, Crete, Greece, October 7-11, **1996**.
11. **V.G. Mavrantzas**, D.N. Theodorou, “From chain chemical structure to polymer melt elasticity: The implementation of new Monte Carlo techniques”, *1st Panhellenic Chemical Engineers’ Conference*, Patras, Greece, May 29-31, **1997**.
12. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N. Theodorou, “From chemical structure to polymer processing: Atomistic simulation of the viscoelasticity of linear polyethylene melts”, *4th Hellenic Polymer Society Symposium (ELEP 1997)*, Patras, Greece, November 20-22, **1997**.
13. **V.G. Mavrantzas**, V.A. Harmandaris, D.N. Theodorou, “Atomistic simulation of the viscoelasticity of linear polyethylene melts”, *1st Hellenic Society of Rheology Meeting*, Heraklion, Greece, August 29-September 2, **1998**.
14. E. Zervopoulou, **V.G.** **Mavrantzas**, D.N.Theodorou, “Atomistic simulation of the solubility of small alkanes in long polyethylene melts”, *2nd Panhellenic Chemical Engineers’ Conference*, Salonica, Greece, May 27-29, **1999**.
15. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N. Theodorou, “Atomistic simulation of the stress relaxation experiment after cessation of steady-state uniaxial elongation”, *2nd Panhellenic Chemical Engineers’ Conference*, Salonica, Greece, May 27-29, **1999**.
16. M. Apostolakis, J. Hatzinicolaou, **V.G.** **Mavrantzas**, “Stress-induced polymer migration effects in the Taylor-Couette device: Numerical calculations with spectral elements”, *2nd Panhellenic Chemical Engineers’ Conference*, Salonica, Greece, May 27-29, **1999**.
17. V.A. Harmandaris, **V.G. Mavrantzas**, D.N.Theodorou, “Atomistic Modeling of Viscoelasticity: Simulation of stress relaxation upon cessation of steady-state elongational flow”`, *Summer School in Polymer Science and Technology*, Psathopirgos, Patras, Greece, September 5-9, **1999**.
18. **V.G. Mavrantzas**, A.N. Beris, “A hierarchical, self-consistent model for the study of surface effects on the structure and rheology of polymer solutons. I) General formulation with application to the flow past a wall, II) Application to an adsorbing surface”, Proceedings, *Interfaces and Colloidal Systems*, Aghia Pelaghia, Heraklion Crete, Greece, September 18-23, **1999**.
19. **V.G. Mavrantzas**, H.C. Öttinger, “GENERIC: A guide for the design of atomistic Monte Carlo simulations for nonequilibrium systems”, *Nonequilibrium Thermodynamics and Complex Fluids*, Oxford, UK, August 14-18, **2000**.
20. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N.Theodorou, “Prediction of the linear viscoelastic properties of long-chain polyethylene melts from detailed atomistic simulations on uniaxially stretched melt configurations”, *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000**.
21. **V.G. Mavrantzas**, A.N. Beris, “Polymer depletion phenomena near a solid surface: Modeling the effect of a shear flow”, *XIII International Congress on Rheology*, Cambridge, UK, August 20-25, **2000.**
22. K.Ch. Daoulas, **V.G. Mavrantzas**, D.Photinos, “Grafted Polymer Melts: Detailed Atomistic Simulation of their Interfacial Structure”, *3rd COST P1 Workshop on Soft Condensed Matter*, Patras, September 22-23, **2000**.
23. M. Apostolakis, **V.G.** **Mavrantzas**,“Polymer diffusion in inhomogeneous flow fields: pseudospectral calculations in the Taylor-Couette geometry”, *35th Annual Meeting of the French Society of Rheology*, Grenoble, October 23-25, **2000**.
24. N.Ch. Karayiannis, **V.G.** **Mavrantzas**,D.N.Theodorou, “Effects of Jump Rate Distribution and Spatial Heterogeneity”, *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000**.
25. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N. Theodorou, “Rheological Properties of Polymer Melts from Molecular Constitution”, *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000.**
26. **V.G. Mavrantzas**,E. Zervopoulou, M. Doxastakis, D.N. Theodorou, “Prediction of Physical Properties of Polymer Melts”, *AIChE Annual Meeting*, Los Angeles, November 13-17, **2000.**
27. I.E. Mavrantza, D. Prentzas, **V.G.** **Mavrantzas**,C. Galiotis, “Detailed atomistic molecular dynamics simulation of the temperature dependence of the IR vibrational spectra of crystalline polyethylene”, *2nd Seminar of the Greek Network of Polymers,* Patras, April 6, **2001**.
28. K. Daoulas,A.F. Terzis, **V.G.** **Mavrantzas**,“Melts of macromolecules grafted on a hard surface or graphite: Detailed atomistic simulation of their interfacial structure”, *3rd Panhellenic Chemical Engineers’ Conference*, Athens, Greece, May 31-June 02, **2001**.
29. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N. Theodorou, “Prediction of the viscoelastic properties of high-molecular weight polymer melts through molecular dynamics atomistic simulations”, *3rd Panhellenic Chemical Engineers’ Conference*, Athens, Greece, May 31-June 02, **2001**.
30. M. Apostolakis, **V.G.** **Mavrantzas**, A.N.Beris, “Polymer diffusion in the Taylor-Couette geometry: Calculation of the time-dependent basic flow with pseudo-spectral elements”, *3rd Panhellenic Chemical Engineers’ Conference*, Athens, Greece, May 31-June 02, **2001.**
31. M. Apostolakis, **V.G.** **Mavrantzas**, A.N. Beris, “Stress-induced migration effects on the viscoelastic Taylor-Couette flow", *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-14, **2001.**
32. V.A. Harmandaris, **V.G. Mavrantzas**,D.N. Theodorou, “Prediction of the rheological properties of long polyethylene melts via atomistic molecular dynamics simulations", *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-14, **2001.**
33. K.Ch. Daoulas, A.F. Terzis, **V.G.** **Mavrantzas**,“Detailed end-bridging Monte Carlo simulations of grafted polyethylene melts”, *Euroconference on Interfaces and Thin Films of Polymers and Colloidal Systems,* Acquafredda di Maratea, Italy, September 8-13, **2001**.
34. **V.G. Mavrantzas,** M. Apostolakis, A.N. Beris, “Stress-induced migration effects in the Taylor-Couette flow: Numerical simulation of the stress-concentration coupling", *73rd Annual Meeting of the Society of Rheology*, Bethesda, Maryland, USA, October 21-25, **2001.**
35. Daoulas, K.;Terzis, A.F.; **Mavrantzas, V.G.,** “Detailed end-bridging Monte Carlo simulations of polymer melts grafted on a solid substrate”, Proceedings*, 5th Hellenic Polymer Society Symposium (ELEP 2001)*, Heraklion, Crete, December 15-17, **2001**.
36. Karayiannis, N.C.; **Mavrantzas, V.G.**; Theodorou, D.N.,“A new method for the rapid equilibration of atomistic macromolecular model systems of a precisely defined chemical architecture”, Proceedings*, 5th Hellenic Polymer Society Symposium (ELEP 2001)*, Heraklion, Crete, December 15-17, **2001**.
37. **V.G. Mavrantzas**, V.A. Harmandaris, D.N. Theodorou, “Atomistic Monte Carlo simulations of the viscoelastic properties of polymer melts”, *4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
38. K.Ch. Daoulas, **V.G. Mavrantzas**,V.A. Harmandaris, K. Foteinopoulou, D.N. Theodorou, “Atomistic Monte Carlo simulations and SCF Calculations of polymers at interfaces”*, 4th GRACM Congress on Computational Mechanics*, Patras, Greece, June 27-29, **2002**.
39. **V.G. Mavrantzas**, A.N. Beris, “Modeling interfacial effects on the conformation and rheology of polymer solutions through a hierarchical, continuum model”, *Chain Molecules at Interfaces, A Symposium to the memory of Jan Scheutjens*, Wageningen University, The Netherlands, August 25-28, **2002.**
40. K.Ch. Daoulas, **V.G.** **Mavrantzas**, “Detailed atomistic Monte Carlo simulation of grafted polymer melts: Thermodynamic, conformational and structural properties”, *Chain Molecules at Interfaces, A Symposium to the memory of Jan Scheutjens*, Wageningen University, The Netherlands, August 25-28, **2002**.
41. N.Ch. Karayiannis, **V.G.** **Mavrantzas**,“A novel Monte Carlo scheme for the detailed simulation of nonlinar H-shaped model polyethylene melts”, *XVIII Panhellenic Conference on Solid State Physics-Materials Science,* Heraklion, Crete, September 15-18, **2002**.
42. K.Ch. Daoulas, **V.G.** **Mavrantzas**,“Detailed atomistic Monte Carlo simulation of grafted polymer melts”, *Euresco,* Spain, 14-19 September, **2002**.
43. V.A. Harmandaris, **V.G. Mavrantzas**, D.N.Theodorou, “Prediction of the viscoelastic properties of polymer from detailed molecular dynamics simulations and comparison against rheological measurements", *3rd Chemical Engineering Conference for Collaborative Research in Eastern Mediterranean (EMCC-3)*, Thessaloniki, Greece, May 13-15, **2003.**
44. K. Foteinopoulou, **V.G.** **Mavrantzas**, J.Tsamopoulos, “Numerical calculation of bubble growth in Newtonian and viscoleastic filaments undergoing stretching”, *4th Panhellenic Chemical Engineers’ Conference*, Patras, Greece, May 29-31, **2003**.
45. K.Ch. Daoulas,A.F.Terzis, **V.G.** **Mavrantzas**,“A novel method for precisely controlling the chain length distribution in atomistic simulations of inhomogeneous and/or anisotropic polymer systems with chain connectivity-altering Monte Carlo algorithms”, *4th Panhellenic Chemical Engineers’ Conference*, Patras, Greece, May 29-31, **2003**.
46. G. Tsolou, **V.G.** **Mavrantzas**, D.N. Theodorou, “Atomistic molecular dynamics simulations of cis-1,4 polybutadiene melts”, *4th Panhellenic Chemical Engineers’ Conference*, Patras, Greece, May 29-31, **2003.**
47. K. Foteinopoulou, **V.G.** **Mavrantzas**, J. Tsamopoulos, “Numerical simulation of bubble growth during filament stretching of pressure-sensitive adhesive materials”, *XIIIth International Workshop on Numerical Methods for non-Newtonian flows”,* Lausanne, Switzerland, June 4-7, **2003**.
48. **V.G. Mavrantzas**, “Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: Detailed atomistic simulation of polymer melt viscoelasticity”, *3rd International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (3rd IWNET)*, Princeton, USA, August 14-17, **2003**.
49. **V.G. Mavrantzas**, “Modeling interfacial effects on the conformation and rheology of polymer solutions through a hierarchical, continuum model”, *3rd International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (3rd IWNET)*, Princeton, USA, August 14-17, **2003**.
50. K. Foteinopoulou, **V.G.** **Mavrantzas**,J. Tsamopoulos, “Numerical Simulation of bubble growth during filament stretching”, *The 5th Euromech Fluid Mechanics Conference*, Toulouse, France, August 24-28, **2003**.
51. K.Ch. Daoulas, **V.G. Mavrantzas**,“Atomistic Monte Carlo simulation studies of polymer melts grafted on solid substrates”, *International Conference on Computational Methods in Sciences and Engineering (ICCMSE 2003)*, Kastoria, Greece, September 12-16, **2003**.
52. V.A. Harmandaris, **V.G.** **Mavrantzas**, D.N.Theodorou, “Molecular Dynamics simulation of the viscoelastic properties of linear polymer melts”, *Polymer Processing Society (PPS)*, Athens, Greece, September 14-17, **2003**.
53. N.Ch. Karayiannis, **V.G.** **Mavrantzas,** D.N. Theodorou, “Study of the segmental dynamics and barrier properties of amorphous PET [poly(ethylene terephthalate)] and PEI [poly(ethylene isophthalate)] through atomistic simulations”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
54. N.Ch. Karayiannis, **V.G. Mavrantzas**,“An advanced Monte Carlo algorithm for the fast equilibration of atomistic models of H-shaped polyethylene melts”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
55. V.A. Harmandaris, **V.G. Mavrantzas**, D.N.Theodorou, “Atomistic molecular dynamics simulation of n-alkane self-diffusion in melts and binary blends”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
56. V.A. Harmandaris, **V.G. Mavrantzas**, D.N.Theodorou, “Atomistic molecular dynamics simulation of the viscoelastic properties of long-chain polyethylene melts: Crossover from Rouse to reptation regime”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
57. K.Ch. Daoulas, **V.G.** **Mavrantzas**, “Detailed atomistic Monte Carlo simulation of long-chain end-grafted polymer melts”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
58. **V.G. Mavrantzas**, H.C. Öttinger, “GENERIC Monte Carlo: A thermodynamically founded Monte Carlo for the hierarchical simulation of complex systems under steady-state flow conditions”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
59. K. Foteinopoulou, **V.G.** **Mavrantzas**, J. Tsamopoulos, “Bubble growth during filament stretching of pressure sensitive adhesive materials”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2003.**
60. K.Ch. Daoulas, **V.G.** **Mavrantzas**,“An atomistic simulation approach to the thermodynamics and structural properties of grafted polymer melts”, *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
61. V.A. Harmandaris, K.Ch. Daoulas, **V.G.** **Mavrantzas**, “Atomistic simulation of the structure and dynamics of the polyethylene/graphite interface”, *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
62. N.Ch. Karayiannis, **V.G. Mavrantzas**,“Detailed atomistic simulation of long-cahin branched polyethylene melts”, *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
63. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, “Thermodynamically founded hierarchical methodologies for the simulation of polymer melts beyond equilibrium: detailed atomistic simulation of polymer melt viscoelasticity”, *3rd International Conference on Computational Modeling and Simulation of Materials: From the Atomistic to the Engineering Scales*, Acireale (Catania), Italy, May 30 – June 4, **2004.**
64. K. Foteinopoulou, **V.G.** **Mavrantzas**, J.Tsamopoulos, “Numerical simulation of bubble growth during filament stretching of Newtonian and viscoelastic fluids”,*4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
65. G. Tsolou, **V.G. Mavrantzas**,“Atomistic simulation of the dynamics of cis-1,4 polyboutadiene and its dependence on pressure and temperature”,*4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
66. N.Ch. Karayiannis, **V.G. Mavrantzas**, “Branch point friction and its role in the dynamics of H-shaped polyethylene melts as probed by long molecular dynamics simulations”, *4th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 27-29, **2004.**
67. N.Ch. Karayiannis, **V.G. Mavrantzas**, “Detailed atomistic simulation of the conformational and dynamic properties of H-shaped polyethylene melts”, *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
68. **V.G. Mavrantzas**, D.N. Theodorou, H.C. Öttinger, “Thermodynamically founded atomistic Monte Carlo for the simulation of polymer melt viscoelasticity”, *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
69. N.Ch. Karayiannis, **V.G. Mavrantzas**,“Detailed atomistic simulation of the conformational and dynamic properties of H-shaped polyethylene melts”, *XIVth International Congress on Rheology,* Seoul, Korea, August 22-27, **2004.**
70. K. Foteinopoulou, **V.G.** **Mavrantzas**, J. Tsamopoulos, “Numerical Simulation of cavitation dynamics in extensional flows of polymeric filaments”, *FLOW 2004 Meeting*, Athens, Greece, November **2004**.
71. N.Ch. Karayiannis, **V.G.** **Mavrantzas**,“Role of branch point friction in the relaxation of H-polymers from detailed, 3μs-long, atomistic molecular dynamics simulations”, *76th Annual Meeting of the Society of Rheology*, Lubock, USA, February 13-17, **2005.**
72. K. Foteinopoulou, **V.G.** **Mavrantzas**, J. Tsamopoulos, “Numerical calculation of the deformation of multiple bubbles in a filament undergoing stretching”,*2nd Annual European Rheology Conference (AERC-2005),* Grenoble, France, April 21-23, **2005.**
73. O. Alexiadis, K.Ch. Daoulas, **V.G.** **Mavrantzas**, “Atomistic Monte Carlo simulation of alkanethiol based self-assembled monolayers on the Au(1,1,1) surface”, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
74. N.Ch. Karayiannis, **V.G. Mavrantzas**, “Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long atomistic molecular dynamics simulations”, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
75. G. Tsolou, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of pressure and temperature effects on cis-1,4 polybutadiene and polyethyene”, *5th Panhellenic Chemical Engineers Conference*, Thessaloniki, Greece, May 26-28, **2005**.
76. V.A. Harmandaris, **V.G.** **Mavrantzas**, “Chain diffusion and mobility in thin films of polyethylene melts adsorbed on graphite through atomistic simulations”, *European Polymer Congress*, Moscow, Russia, June 27-July 1, **2005.**
77. K. Foteinopoulou, **V.G.** **Mavrantzas**, J.Tsamopoulos, “Numerical simulation of multi-bubble growth in filaments undergoing stretching”,*5th GRACM International Congress on Computational Mechanics,* Limassol, Cyprus, June 29-July 1, **2005.**
78. N.Ch. Karayiannis, **V.G.** **Mavrantzas**, “Calculation of branch point friction and chain reptation time of H-shaped polyethylene melts from long atomistic molecular dynamics simulations”, CECAM Meeting on: *Modeling and Simulation of Entangled polymeric liquids*, Lyon, France, July 18-21, **2005.**
79. **V.G. Mavrantzas**, K. Foteinopoulou, J. Tsamopoulos, “On the deformation and translation of multiple bubbles in a viscoelastic filament undergoing stretching”,SOR 77th Annual Meeting, Vancouver, British Columbia, Canada, October 16-20, **2005**.
80. V. Soni, J. Abildskov, G. Jonsson, R. Gani, N. Karayiannis, **V.G. Mavrantzas**, “*Model based design of structured polymers using the reverse design approach*”, *AIChE Annual Meeting*, San Francisco, USA, November 16-21, **2005.**
81. T. Ionescu, B.J. Edwards, V.G. Mavrantzas, *“*Atomistic simulation of energetic and entropic elasticity in short-chain polyethylenes*”* *AIChE Annual Meeting*, Cincinnati, USA, Oct. 30-Nov. 4, **2005.**
82. N.Ch. Karayiannis, **V.G. Mavrantzas**, “Hierarchical modeling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations”, *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
83. G. Tsolou, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of the temperature and pressure dependence of local and terminal relaxation in amorphous polyethylene and *cis*-1,4 polybutadiene”, *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
84. **V.G. Mavrantzas**, A.N. Beris, “Continuum formulation of the Scheutjens-Fleer lattice statistical theory for homopolymer adsorption from solution”, *231st ACS National Meeting*, Atlanta, USA, March 26-30, **2006**.
85. G. Tsolou, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of the temperature and pressure dependence of local and terminal relaxation in *cis*-1,4 polybutadiene”, *3rd Annual European Rheology Conference (AERC 2006)*, Hersonissos, Crete, Greece, April 27- 29, **2006**.
86. K. Foteinopoulou, N.Ch. Karayiannis, **V.G. Mavrantzas**, M.Kröger, “Topological analysis of polyethylene melts: Results from a hierarchical modeling approach combining atomistic Monte Carlo and long molecular dynamics simulations followed by a direct analysis of entanglements (poster)”, *3rd Annual European Rheology Conference (AERC 2006)*, Hersonissos, Crete, Greece, April 27- 29, **2006**.
87. T. Ionescu, B.J. Edwards, D.J. Keffer, **V.G. Mavrantzas**, “Thermodynamics of non-isothermal polymer melts: Experiment, theory and simulation”, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
88. N.Ch. Karayiannis, **V.G. Mavrantzas**, “Atomistic simulation of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt (poster)”, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
89. K. Foteinopoulou, N.Ch. Karayiannis, **V.G. Mavrantzas**, M.Kröger, “Primitive path identification and entanglement statistics in polymer melts: results from a direct topological analysis on atomistically detailed polyethylene models”, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
90. V. Dimitriadis, N.Ch. Karayiannis, **V.G.** **Mavrantzas**, E.Chiotellis, D. Mouratides, C.D. Kiparissides, “Structure and dynamics of polyethylene melts bearing short chain branches frequently spaced along their backbone as revealed from atomistic simulations (poster)”, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
91. G. Tsolou, **V.G.** **Mavrantzas**, “Atomistic molecular dynamics simulation of the temperature and pressure dependences of local and terminal relaxations in cis-1,4-polybutadiene”, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (4th IWNET)*, Rhodes, Greece, September 3-7, **2006.**
92. V. Soni, J. Abildskov, G. Jonsson, R. Gani, N.Ch. Karayiannis, **V.G. Mavrantzas**, “Multiscale modeling property for design of polymer based products”, *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
93. T. Ionescu, B.J. Edwards, D.J. Keffer, **V.G. Mavrantzas**, “Thermodynamics of non-isothermal polymer melts: Experiment, theory and simulation”, *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
94. R. Khare, O. Alexiadis, **V.G. Mavrantzas**, A. Baljon, “Monte Carlo simulations of the glass transition in polyethylene”, *AIChE Annual Meeting*, San Francisco, USA, Nov. 12 - 17, **2006.**
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188. P.V. Alatas, **V.G. Mavrantzas**, “Applications of a thermodynamic, non-linear quantum master equation to a three-level and a harmonic oscillator system coupled with two heat baths”, *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
189. F.D. Tsourtou, O. Alexiadis, **V.G. Mavrantzas**, V. Kolonias, E. Housos, “Atomistic simulation of the bulk phase self-assembly of semifluorinated alkanes”, *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
190. E.N. Skountzos, O. Alexiadis, K. Kasidiaris, **V.G. Mavrantzas**, “Atomistic simulation of the structural and thermodynamic properties of organic semiconducting polymers”, *28th European Symposium on Applied Thermodynamics (ESAT 2015)*, Athens, Greece, June 11-14, **2015**.
191. C. Baig, **V.G. Mavrantzas**, “Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble”, *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015),* Hilvarenbeek, The Netherlands, July 6-10, **2015**.
192. P. Stephanou, **V.G. Mavrantzas**, G.C. Georgiou, “A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics”, *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015),* Hilvarenbeek, The Netherlands, July 6-10, **2015**.
193. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, “Structural, conformational, dynamic and topological properties of ring poly(ethylene oxide) melts from molecular dynamics simulations and compasrion with experimental data”, *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.
194. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, “Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites”, *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.
195. P.G. Mermigkis, D.G. Tsalikis, **V.G. Mavrantzas**, “Prediction of the effective diffusivity of water inside CNT-based PMMA membranes, *8th GRACM International Congress on Computational Mechanics,* Volos, Greece, July 12-15 **2015**.
196. P.S. Stephanou, I.Ch. Tsimouri, **V.G. Mavrantzas**, “Flow-induced orientation and stretching of entangled polymers in the framework of non-equilibrium thermodynamics”, *20th Anniversary Meeting of the European Society of Rheology*, ETH-Zurich, Switzerland,March 31 - April 1, **2016**.
197. D.G. Tsalikis, **V.G. Mavrantzas**, “Topological constraints in polymer rings”, *PRACE Scientific and Industrial Conference (PRACE Days16)*, Budapest, Hungary, May 10-12, **2016**.
198. F. Tsourtou, **V.G. Mavrantzas**, “Optimized Atomistic Monte Carlo and Molecular Dynamics Algorithms for simulating self-assembly in soft matter”, *PRACE Scientific and Industrial Conference (PRACE Days16)*, Budapest, Hungary, May 10-12, **2016**.
199. E.N. Skountzos, **V.G. Mavrantzas**, “Large-scale atomistic Molecular Dynamics simulation study of polymergraphene nanocomposites”, *PRACE Scientific and Industrial Conference (PRACE Days16)*, Budapest, Hungary, May 10-12, **2016**.
200. V. Vasilev, E.N. Skountzos, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Predicting the fractal-like structure of SiO2 nanoparticles through molecular dynamics simulations using the potential of mean force”, *MaP Graduate Symposium*, ETH-Zurich, Switzerland, June 9, **2016**.
201. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, “Geometric analysis of ring-ring threading events in melts of ring polymers and their connection with the slow relaxation modes*”, XVIIth International Congress on Rheology (ICR 2016)*, Kyoto, Japan, August 8 - 13, **2016**.
202. P. Alatas, D. Tsalikis, **V.G. Mavrantzas**, “Molecular dynamics simulation of the structure and self-diffusion of short linear and cyclic n-alkanes in melt and blends”, *2nd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, September 23, **2016**.
203. P.S. Stephanou, D.G. Tsalikis, **V.G. Mavrantzas**, “Multiscale modelling approach to the rheological behavior of polymer nanocomposites: Nonequilibrium thermodynamics modeling coupled with NEMD simulations”, *8th International Conference on Multiscale Materials Modeling (MMM-2016)*, Dijon, France, October 9-14, **2016**.
204. P.V. Alatas, D. G. Tsalikis, **V.G. Mavrantzas**, “Comparison of the conformational and dynamic properties between ring and linear poly(ethylene oxide) melts from molecular dynamics simulations in the crossover regime from unentangled to entangled”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
205. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of water mobility inside Carbon Nanotubes embedded in a PMMA matrix”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
206. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, “Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
207. P.S. Stephanou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Non-equilibrium thermodynamics modelling and atomistic simulation of polymer nanocomposites”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
208. D.G. Tsalikis, **V.G. Mavrantzas**, D. Vlassopoulos, “Geometric analysis of threading events in melts of ring polymers and their connection with the slow relaxation modes”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
209. I.Ch. Tsimouri, Ch.Κ. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, “Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
210. F.D. Tsourtou, **V.G. Mavrantzas**, “Atomistic Monte Carlo and Molecular Dynamics Algorithms for the simulation of self-assembly in soft matter”, *11th* *Hellenic Polymer Society Conference (ELEP 2016)*, Heraklion, Crete, Greece, November 3-5, **2016**.
211. E.N. Skountzos, **V.G. Mavrantzas**, S.E. Pratsinis, “From atoms to primary particles to agglomerates: Hierarchical modeling of the fractal dimensions of nanoparticles”, *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
212. E.N. Skountzos, **V.G. Mavrantzas**, C. Tsitsilianis, “Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites”, *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
213. D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, “Computational study of microscopic dynamics in Polyethylene Glycol melts filled with Silica Nanoparticles and comparison with experimental data”, *2016 MRS Fall Meeting & Exhibit*, Boston, USA, November 27 - December 2, **2016**.
214. P.S. Stephanou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations”, *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
215. I.Ch. Tsimouri, C.K. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, “Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics”, *11th Annual European Rheology Conference (AERC-2017)*, Copenhagen, Denmark, April 3-6, **2017**.
216. D.G. Tsalikis, G.D. Papadopoulos, **V.G. Mavrantzas**, “Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data”, *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
217. F. Tsourtou, **V.G. Mavrantzas**, “Optimized Monte Carlo and Molecular Dynamics algorithms for modelling the self-organization of two classes of materials: semifluorinated alkanes and semiconducting polymers based on thiophenes”, *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
218. E.N. Skountzos, **V.G. Mavrantzas**, “Atomistic simulation of pyrene functionalized α,ω-PMMA as dispersing agent of graphene for the fabrication of polymer nanocomposites”, *PRACE Scientific and Industrial Conference (PRACEdays17)*, Barcelona, Spain, May 16-18, **2017**.
219. P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, “Molecular dynamics simulation of the differences in the conformational and dynamic properties between and linear polyethylene oxide melts in the crossover region from unentangled to entangled”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
220. A. Spyrogianni, K.K. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Brownian dynamic simulation of the settling rate of fractal-like nanoparticle agglomerates”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
221. D. Mallios, D.G. Tsalikis, **V.G. Mavrantzas**, “Self-assembly of amphiphile peptides into nanostructures through detailed molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
222. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, “Study of water molecule mobility in carbon nanotubes embedded in a PMMA matrix”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
223. D. Mintis, P.V. Alatas, D.G. Tsalikis, **V.G. Mavrantzas**, “Conformational transition of poly(ethylene-imine) in aqueous solution at different protonation states and its role in the formation of complex coacervate elucidated from Atomistic Molecular Dynamics Simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
224. C.Κ. Georgantopoulos, I.Ch. Tsimouri, P.S. Stephanou, **V.G. Mavrantzas**, “Development of state-of-the-art constitutive rheological models for entangled polymeric fluids using principles of nonequilibrium thermodynamics”,*11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
225. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, “On the effect of end-functionalized groups on the dynamics of polymer melt nanocomposites through molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
226. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, “Modelling of polymer nanocomposite melts based on principles of nonequilibrium thermodynamics and on the findings of detailed nonequilibrium molecular dynamics simulations”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
227. I.Ch. Tsimouri,P.S. Stephanou, **V.G. Mavrantzas**, “A constitutive rheological model for the blodod from nonequilibrium thermodynamics”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
228. F.D. Tsourtou, **V.G. Mavrantzas**, “Atomistic Monte Carlo and Molecular Dynamics simulation of nanostructured semiconducting polymers and polypeptides”, *11th* *Panhellenic Chemical Engineers Conference*, Salonica, Greece, May 25-27, **2017.**
229. E.N. Skountzos, D.G. Tsalikis, **V.G. Mavrantzas**, “Molecular simulation of PMMA-graphene and PEO-silica polymer nanocomposites in full atomistic detail”, *SCIMEETING Europe, Materials Modellig and Simulations Conference*, Athens, Greece, June 21-23, **2017**.
230. F. Tsourtou, S. Peroukidis, and **G. Mavrantzas**, “Monte Carlo and Molecular Dynamics simulation of liquid-crystalline phases of oligothiophenes using a united-atom model”, *14th European Conference on Liquid Crystals* *(ECLC 2017)*, Moscow, Russia, June 24-30, **2017**.
231. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, “The effect of organics and humidity on the structure of atmospheric nanoparticles: A molecular dynamics simulation study”, *20th International Conference on Nucleation and Atmospheric Aerosols (ICNAA 2017)*, Helsinki, Norway, June 25-39, **2017**.
232. P.S. Stephanou, D.G. Tsalikis, E.N. Skountzos, **V.G. Mavrantzas**, “Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations”, *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
233. D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Ring polymers: scaling laws and topological interactions based on detailed molecular dynamics simulations”, *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
234. P.S. Stephanou, **V.G. Mavrantzas**, “Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level”, *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
235. I.Ch. Tsimouri, C.Κ. Georgantopoulos, P.S. Stephanou, **V.G. Mavrantzas**, “Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics”, *8th International Meeting of the Hellenic Society of Rheology (HSR 2017)*, Limassol, Cyprus, July 12-14, **2017.**
236. K.S. Karadima, **V.G. Mavrantzas**, S.N. Pandis, “Molecular dynamics simulation of atmospheric nanoparticles: local structure and morphology”, *European Aerosol Conference (EAC 2017)*, Zurich, Switzerland, August 27-September 01, **2017**.
237. D.G. Tsalikis, **V.G. Mavrantzas**, “Microscopic dynamics and topology of polymer rings immersed in a host matrix of longer linear polymers: Results from a detailed molecular dynamics simulation study and comparison with experimental data”, *Ring Polymers: Focused Workshop,* Heraklion, Crete, September 25-27, **2017**.
238. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Mobility and Sedimentation of Agglomerates with Polydisperse Primary Particles”, *2017 Conference of the Americal Association for Aerosol Research (2017 AAAR)*, Raleigh, North Carolina, October 16-20, **2017**.
239. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Sedimentation of Agglomerates Consisting of Polydisperse Nanoparticles”, *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
240. A. Spyrogianni, K.S. Karadima, E. Goudeli, **V.G. Mavrantzas**, S.E. Pratsinis, “Settling rate of agglomerates consisting of polydisperse primary particles by Brownian Dynamics”, *AIChE Annual Meeting*, Minneapolis, USA, October 29 - November 03, **2017**.
241. D.G. Tsalikis, **V.G. Mavrantzas**, “Melt rheology of ring poly(ethylene oxide) melts and comparison with experimental data”, *12th Annual European Rheology Conference (AERC-2018)*, Sorrento, Italy, April 17-20, **2018**.
242. **V.G. Mavrantzas**, P.V. Alatas, H.C. Öttinger, “Third-order perturbation expansion of the two-point correlation function of the dissipative quantum φ4 theory”, *8th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2018),* Sint-Michielsgestel, The Netherlands, July 1-6, **2018**.
243. D. Mintis, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of weak polyelectrolytes in water”, *12th International Symposium on Polyelectrolytes (ISP2018)*, Wageningen, The Netherlands, August 26-31, **2018**.
244. F.D. Tsourtou, K. Kardima, **V.G. Mavrantzas**, “Atomistic Monte Carlo: A powerful technique for simulating self-assembly in polypeptides”, *BioExcel 2nd SIG Meeting: “Advanced Simulations for Biomolecular Research” @ ECCB 2018*, Athens, Greece, September 8, **2018**.
245. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Conformational and dynamic properties of DNA minicircles in aqueous solution from atomistic molecular dynamics simulations”, *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
246. P.G. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, “Conformational, dynamic, and permeability properties of atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposites from molecular simulations”, *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
247. D.G. Tsalikis, **V.G. Mavrantzas**, “Conformation and dynamics of ring polymers in dilute solutions of linear matrices: Results from a systematic molecular dynamics simulation study and comparison with experimental data”, *12th Hellenic Polymer Society International Conferemce (ELEP 2018)*, Ioannina, Greece, September 30-October 3, **2018**.
248. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Atomistic simulation of DNA minicircles in aqueous solution”, *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
249. F.D. Tsourtou, K.S. Karadima, **V.G. Mavrantzas**, “Self-assembly in polypeptides with atomistic Monte Carlo”, *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
250. D. Mintis, **V.G. Mavrantzas**, “ Molecular dynamics simulation of the weak polyelectrolytes poly(ethylene-imine), poly(acrylic acid) and poly(N,N-dimethylaminoethyl methacrylate): Effect of salt, pH, temperature, branching and chain size”, *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
251. P. Mermigkis, E.N. Skountzos, **V.G. Mavrantzas**, “Conformational, dynamic, and permeability properties of atactic poly(methyl methacrylate) - carbon nanotube (PMMA-CNT) nanocomposites studied through molecular dynamics simulations”, *4th Workshop of Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, October 31, **2018**.
252. A.J. Tsamopoulos, D.G. Tsalikis, **V.G. Mavrantzas**, “Shear rheology of marginally entangled ring-linear poly(ethylene oxide) blends through nonequilibrium atomistic molecular dynamics simulations”, *12th Annual European Rheology Conference (AERC-2019)*, Portorož, Slovenia, April 8-11, **2019**.
253. T. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Conformational and transport properties of DNA minicircles in dilute aqueous solutions: Detailed atomistic molecular dynamics simulation study”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
254. D.G. Mintis, **V.G. Mavrantzas**, “All atomistic molecular dynamics study of the effect of pH and molecular weight on structure and dynamics of the weak polyelectrolyte poly(acrylic acid)”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
255. A.J. Tsamopoulos, A. Katsarou, D.G. Tsalikis, **V.G. Mavrantzas**, “Nonequilibrium molecular dynamics simulation of marginally entangled linear-ring polymer belnds”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
256. D.G. Mintis, D. Rigou, **V.G. Mavrantzas**, “Detailed molecular dynamics simulation study of the phase boundary for complex coacervation between poly(acrylic acid) and poly(N,N-dimethyl amino ethyl methacrylate) (poster presentation)”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
257. T. Alexiou, E. Kriti, D. Loukas, **V.G. Mavrantzas**, “Atomistic molecular dynamics simulation of the diffusive behavior of short linear DNA molecules in dilute aqueous solutions: Comparison with experiments and theoretical models (poster presentation)”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
258. A.F. Katsarou, A.J. Tsamopoulos, D.G. Tsalikis, **V.G. Mavrantzas**, “Dynamic heterogeneity ad topological intearctions in ring-linear polymer blends under flow (poster presentation)”, *12th* *Panhellenic Chemical Engineers Conference*, Athens, May 29-31, **2019**.
259. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Conformational and transport properties of small circular DNA molecules in dilute solution: A detailed molecular dynamics simulation study”, *Frontiers in Polymer Science 2019*, Budapest, Hungary, June 05-08, **2019**.
260. T.S. Alexiou, E. Kriti, D. Loukas, **V.G. Mavrantzas**, “ Atomistic molecular dynamics simulation of the diffusion dynamics of short linear DNA molecules: comparison with experimental data and theoretical models (poster presentation)”, *Frontiers in Polymer Science 2019*, Budapest, Hungary, June 05-08, **2019**.
261. T.S. Alexiou, D.G. Tsalikis, P.V. Alatas, **V.G. Mavrantzas**, “Conformational and transport properties of small circular and linear DNA molecules in dilute solution: A detailed molecular dynamics simulations study”, *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
262. D.G. Tsalikis, P.V. Alatas, T.S. Alexiou, **V.G. Mavrantzas**, “Shear rheology of marginally entangled ring polymer melts through non-equilibrium atomistic molecular dynamics simulations”, *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
263. D.G. Tsalikis, E.N. Skountzos, P.S. Stephanou, **V.G. Mavrantzas**, “On the role of chain end-functional groups on microscopic structure and dynamics of polymer nanocomposites (poster presentation)”, *European Polymer Congress* (*EPF 2019)*, Hersonissos Heraklion Crete, Greece, June 9-14, **2019**.
264. D.G. Tsalikis, A.J. Tsamopoulos, A. Katsarou, **V.G. Mavrantzas**, “Steady shear flow of marginally entangled ring polymer melts through nonequilibrium molecular dynamics simulations”, *9th International Meeting of the Hellenic Society of Rheology (HSR 2019)*, Pythagorion, Samos, Greece, June 23-27, **2019**.
265. P.S. Stephanou, I.Ch. Tsimouri, G.C. Georgiou, **V.G. Mavrantzas**, “Understanding the rheological behaviour of blood from a non‐equilibrium thermodynamics perspective”, *9th International Meeting of the Hellenic Society of Rheology (HSR 2019)*, Pythagorion, Samos, Greece, June 23-27, **2019**.

**INVITED LECTURES**

1. “*Atomistic simulation of the viscoelasticity of unentangled polymer melts*”, Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2000**.
2. “*Modeling the rheology of polymer melts through multiscale modeling*”, Dow Chemicals, Midland, December **2000**.
3. “*Hierarchical modeling of the rheology of polymer melts*”, CECAM-SIMU Workshop, Multiscale Modeling of Materials, Heraklion, Crete, July **2001**.
4. *“Atomistic simulation of polymer melts off equilibrium using principles of irreversible thermodynamics”*, CPERI-CERTH, Salonica, October **2001**.
5. *“Molecular simulations of polymers with emphasis on their viscoelasticity*”, 5th Panhellenic Conference on Polymers, Heraklion, Crete, December 15-17, **2001**.
6. *“A hierarchical model for the rheology of polymers in confined geometries”,* Institute for Polymers, Department of Materials, ETH, Zürich, Switzerland, February **2002**.
7. “*Polymer melts grafted on a solid substrate or graphite: Detailed atomistic simulation of their interfacial properties and 2H-NMR spectrum*”, XVIII Panhellenic Conference on Solid State Physics-Materials Science, Heraklion, Crete, September 15-18, **2002**.
8. “*Atomistic simulations of polymers at multiple time and length scales*”, Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, March **2003**.
9. “*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*”, 1st Mainz Materials Simulation Days (MMSD 2005), Max-Planck Institute for Polymer Research (MPI-P), Mainz, Germany, June 8-10, **2005**.
10. “*Hierarchical modelling of polymers with a non-linear molecular architecture: Calculation of branch point friction and chain reptation time of an H-shaped polyethylene melt from detailed atomistic simulations*”, Japan Society of Technology (JST) Symposium: “Towards Multi-scale Modeling in Soft Matter”, Tokyo, Japan, June 21-22, **2005**.
11. *Multi-scale modelling of polymers with a non-linear molecular architecture*”, Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 5-8, **2006**.
12. “*Simulation of polymers with a non-linear molecular architecture*”, ΕΚΕΤΑ-ΙΤΧΗΔ, February 3, **2006**.
13. “*Multi-scale modeling of polymers with a non-linear molecular architecture*”, Keynote lecture, International Workshop on Mesoscale and Multiscale Description of Complex Fluids, Prato, Italy, July 5-8, **2006**.
14. *“Thermodynamically guided atomistic Monte Carlo simulation of polymer melts beyond equilibrium”,* International Workshop on Multi-scale Modeling and Simulation of Complex Fluids, Maryland, USA, April 13-19, **2007.**
15. *“Polymer melt viscoelasticity: What can we learn from molecular simulations”,* Department of Materials Science, University of Crete, Heraklion, Crete, May 25, **2007**.
16. *“Polymer melt viscoelasticity: What can we learn from molecular simulations”,* Department of Applied Physics, University of Eindhoven, Eindhoven, The Netherlands, October 1, **2007**.
17. *“Hierarchical Modeling of Polymers: From the atomistic to the meso- to the macro-scale”,*ENPC, Paris, November 26, **2007**.
18. *“Modeling in nanomaterials: The Monte Carlo Method”,* International school on Nanostructure materials and membranes modeling and simulation*,* FORTH-ICE/HT, Patras, June 18-27, **2008**.
19. *"Atomistic Monte Carlo methodology for generating realistic flows of polymers guided by principles of non-equilibrium thermodynamics",* Polymer Physics Gordon Conference, Salve Regina University, Rhode Island, USA, June 29 - July 4, **2008.**
20. *“Hierarchical modeling of polymers at equilibrium and beyond-equilibrium conditions with emphasis on their mechanics and viscoelasticity”,* DSM-Sabic R&D, The Netherlands, September 26, **2008**.
21. “*Hierarchical modeling of polymers at equilibrium and beyond equilibrium conditions with emphasis on viscoelasticity*”, International seminar on Multi-scale modeling and simulation, Trondheim, Norway, October 13-14, **2008**.
22. “*Multiscale simulation of polymer melt viscoelasticity guided from non-equilibrium statistical thermodynamics: Atomistic Non-Equilibrium Molecular Dynamics coupled with Monte Carlo in an expanded statistical ensemble*”, 6th International Discussion Meeting on Relaxations in Complex Systems, Rome, Italy, August 30 - September 5, **2009**.
23. “*Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model*”, Theory and Computer Simulation of Polymers", Moscow, Russia, May 31 - June 6, **2010**.
24. *“Modeling polymer melt viscoelasticity: Quantifying chain reptation in entangled polymer melts through a novel topological and dynamical mapping of atomistic simulation results onto the tube model*”, International Workshop on Novel Simulation methods in Soft matter Systems (NSASM-2010)”, Dresden, Germany, September 20-24, **2010**.
25. *“Atomic and electronic structure of polymer organic semiconductors: What we can learn from computer simulations at different scales*”, 9th Hellenic Polymer Society Symposium (ELEP 2012), Thessaloniki, Greece, November 29-December 01, **2012**.
26. *“Interfacing molecular simulations with theories of polymer dynamics: the case of entangled polymer melts and polymer rings”,* Department of Materials Science, University of Crete, Heraklion, Crete, March 01, **2013**.
27. *“Topological interactions in ring poly(ethylene oxide) melts and their correlation with conformational and rheological properties: A computer simulation study”,* Ring Polymers: Advances and Applications*,* Heraklion, Crete, July 12-15, **2015**.
28. *Simulation of polymer melts beyond equilibrium using a non-dynamic method (GENERIC Monte Carlo) in an expanded ensemble*, Technical University of Eindhoven, Department of Mechanical Engineering, April 19,**2016.**
29. *Using nonequilibrium thermodynamics to extend atomistic Monte Carlo simulations of polymers beyond equilibrium*, Multiscale Simulation Methods for Soft Matter Systems, Darmstadt, Germany, October 4-6, **2016**.
30. *Atomistic Monte Carlo simulation of self-assembly in soft matter systems,* SCIMEETING Europe, Materials Modellig and Simulations Conference, Athens, Greece, June 21-23, **2017**.
31. *Fundamentals of Molecular Simulations*, Advances in the Mechanics and Chemistry of Adshesion: Training School in the course of the European Marie-Curie Training Project BioSmartTrainee, Paris, France, September 13-15, **2017**.
32. *Microscopic dynamics and threadings in ring polymers: A detailed computer simulation study*, Ring Polymers: Focused Workshop*,* Heraklion, Crete, September 25-27, **2017**.
33. *Molecular modelling of materials: making a difference in industry,* Plastics Update, 2nd edition, Fribourg, Switzerland, November 9, **2017**.
34. *Multiscale materials modelling with emphasis to polymers: making a difference in industry,* International Workshop on Smart Models for Smart Materials (SM)2, March 27-28, Fraunhofer-Zentrum, Kaiserslautern, **2019**.

# TEACHING

### Undergraduate Courses

1. “*Introduction to informatics I*”, Laboratory, Department of Materials Science, University of Patras, Fall **2000** (with Dr. A. Terzis, Dr. E. Serpi, Dr. A. Vanakaras).
2. “*Introduction to informatics II*”, Department of Materials Science, University of Patras, Spring **2002** (with Dr. A. Vanakaras, and Dr. M. Paspalakis).
3. “*Physical Chemistry ΙΙ*”, Department of Chemical Engineering, University of Patras, Spring **2003**, Spring **2004**, Spring **2005**, Spring **2006**, Spring **2007,** Spring **2009**, Spring **2010**, Spring **2011,** Spring **2013**.
4. “*Physical Chemistry*”, Department of Chemical Engineering, University of Patras, Fall **2017** (with Prof. D. Kondarides), Fall **2018** (with Prof. D. Kondarides), Fall **2019** ((with Prof. D. Kondarides).
5. “*Special Topics of Physical Chemistry*”, Department of Chemical Engineering, University of Patras, Fall **2003**, Fall **2004**, Fall **2005**.
6. *“Polymer rheology”*, Department of Chemical Engineering, University of Patras, Fall **2006**, Fall **2007**, Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**, Fall **2012**.
7. “*Mass, Energy and Entropy Balances*”, Department of Chemical Engineering, University of Patras, Fall **2019** (with Prof. D. Spartinos).

### Graduate Courses

1. “*Computer simulation of polymers*”, Interdepartmental Programme of Graduate Studies on “Polymer Science and Technology”, University of Patras, Spring **1999,** Spring **2000,** Spring **2002** (with Dr. A. Terzis and Prof. D. Theodorou).
2. *Molecular Simulation and Statistical Mechanics,* Department of Chemical Engineering, University of Patras, Spring **2003**, Spring **2005**, Spring **2007**, Spring **2009**, Spring **2011**, Spring **2012**, Spring **2018**, Spring **2019**.
3. “*Polymer rheology and processing*”, Interdepartmental Programme of Graduate Studies on “Polymer Science and Technology”, University of Patras, Fall **2000**, Spring **2002** (with Prof. J. Tsamopoulos).
4. “*Graduate Thermodynamics*”, Department of Chemical Engineering, University of Patras, Fall **2003**, Fall **2004**, Fall **2005**, Fall **2006**, Fall **2007,** Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**.
5. “*Polymer rheology*”, Inter-departmental Programme of Graduate Studies in “Polymer Science and Technology”, University of Patras, Fall **2003**, Fall **2004**, Fall **2005**, Fall **2006**, Fall **2007,** Fall **2008,** Fall **2009**, Fall **2010**, Fall **2011**, Fall **2012,** Fall **2017** (with Dr. D.G. Tsalikis).
6. *“Polymer rheology”*, Department of Chemical Engineering & Inter-Department Programe of Graduate Studies in “Polymer Science and Technology”, University of Patras, Fall **2018** (with Dr. D.G. Tsalikis), Fall **2019** (with Dr. D.G. Tsalikis).
7. “*Advanced Course on: Molecular simulation of Complex Chemical Systems with Emphasis to Practical Applications*”, Danish Technical University (DTU), Lyngby, Denmark, June 28-July 9, **2010**.
8. *“Theory of Open Quantum Systems”,* A crash course based on the book by Breuer-Petruccione: “The Theory of Open Quantum Systems (Clarendon, Oxford University Press, 2002)”, Department of Materials Science, ETH-Z, Switzerland, June 25-July 20, **2012**.

# TEACHING AT ETH-Z

1. *“Introduction to Nanomaterials Engineering (INE)”,* Department of Mechanical Engineering, ETH Zurich,Fall **2016** (with Prof. S.E. Pratsinis and Dr. K. Wegner), Fall **2017** (with Dr. R. Büchel), Fall **2018** (with Prof. S.E. Pratsinis), Fall **2019** (with Prof. S.E. Pratsinis).
2. *“Mass Transfer”,* Department of Mechanical Engineering, ETH Zurich, Fall **2018** (with Prof. S.E. Pratsinis), Fall **2019** (with Prof. S.E. Pratsinis).
3. *“Micro- & Nano-Particle Technology (MNP)”,* Department of Mechanical Engineering, ETH Zurich,Fall **2018** (with Prof. S.E. Pratsinis), Fall **2019** (with Prof. S.E. Pratsinis).

**STUDENT ADVISEMENT AS RESEARCHER AT FORTH-ICE/HT**

### Diploma Thesis students

1. John Hatzinikolaou (academic advisor: Prof. D. Theodorou, graduated in 1999)
2. Michalis Apostolakis (academic advisor: Prof. D. Theodorou, graduated in 1999)
3. Dimitris Prentzas (academic advisor: Prof. C. Galiotis, graduated in 1999)
4. Costas Doulas (academic advisor: Prof. D. Theodorou, graduated in 2002)
5. Aggeliki Yianoussaki (academic advisor: Prof. D. Theodorou, graduated in 2002)

### Masters’ Degree students

1. Dimitra Aggelopoulou (academic advisor: Prof. D. Theodorou, graduated in 2000)
2. Michalis Apostolakis (academic advisor: Prof. D. Theodorou, graduated in 2000)
3. Ioanna-Elisavet Mavrantza (academic advisor: Prof. C. Galiotis, graduated in 2000)
4. Georgia Schismenou (academic advisor: Prof. D. Theodorou, graduated in 2001)
5. Georgia Tsolou (academic advisor: Prof. D. Theodorou, graduated in 2001)

### Ph.D. students

1. Evangelia Zervopoulou (academic advisor: Prof. D. Theodorou, graduated in 2000)
2. Vagelis Harmandaris (academic advisor: Prof. D. Theodorou, graduated in 2001)
3. Nikos Karayiannis (academic advisor: Prof. D. Theodorou, graduated in 2002)
4. Kostas Daoulas (academic advisor: Prof. D. Photinos, graduated in 2003)

**STUDENTS ADVISEMENT, DEPARTMENT OF CHEMICAL ENGINEERING, UNIVERSITY OF PATRAS**

### Diploma Thesis students

1. Pavlos Stephanou (graduated in 2006)
2. Eva Lionta (graduated in 2010)
3. Vasilis Georgilas (graduated in 2010)
4. Eirini Goudeli (graduated in 2012)
5. Katiana Efstratiou (graduated in 2013)
6. Aggeliki Chatzintouna (graduated in 2013)
7. Apostolos Ziovas (graduated in 2014)
8. Ioanna Mavrikou (graduated in 2014)
9. Andreas Doukas (graduated in 2014)
10. George Papadopoulos (graduated in 2014)
11. Christos Tsakonas (graduated in 2014)
12. Lina Aggelaki (graduated in 2015)
13. Artemis Charalampidou (graduated in 2015)
14. Maria Koukouta (graduated in 2015)
15. Spyros Agorgiannitis (graduated in 2016)
16. Dimitris Mallios (graduated in 2016)
17. Ioanna Tsimouri (graduated in 2016)
18. Eleni Xygki (graduated in 2017)
19. Costantinos Kasidiaris (graduate in 2018)
20. Christos Georgantopoulos (graduate in 2018)
21. Eleni Chousa (graduate in 2018)
22. Alexandros Tsamopoulos (graduate in 2019)
23. Despoina Rigou (graduate in 2019)
24. Anna Katsarou (graduate in 2019)
25. Evaggelia Kriti (2017- to date)
26. Dimitris Loukas (2018-to date)
27. Panagiotis Cargados (2019 – to date)
28. Aspasia Triantafyllou (2019 – to date)

### Masters’ Degree students

1. Antigoni Theodoratou (graduated in 2010)
2. Nikos Stratikis (graduated in 2011)
3. Thanasis Koukoulas (graduated in 2012)
4. Elena Karahaliou (graduated in 2012)
5. Flora Tsourtou (graduated in 2013)
6. Emmanouil Skountzos (graduated in 2013)
7. Panagiotis Alatas (graduated in 2013)
8. Takis Mermigkis (graduated in 2014)
9. George Papadopoulos (graduated in 2018)
10. Ioanna Tsimouri (graduated in 2018)

### Ph.D. students

1. Katerina Foteinopoulou (co-advisement with Prof. J. Tsamopoulos and C. Toprakcioglou, graduated in 2005)
2. Georgia Tsolou (graduate in 2005)
3. Orestis Alexiadis (graduated in 2007)
4. Pavlos Stephanou (graduated in 2011)
5. Alexandros Anastassiou (graduated in 2013)
6. Flora Tsourtou (graduated in 2019)
7. Emmanouil Skountzos (2013- to date)
8. Panagiotis Alatas (2013- to date)
9. Takis Mermigkis (2015- to date)
10. Dimitris Mintis (2016- to date)

### Post-Doctoral Collaborators

* + - 1. Nikos Karayiannis (2002-2006)
      2. Vagelis Harmandaris (2003-2005)
      3. Kostas Daoulas (2003-2005)
      4. Katerina Foteinopoulou (2005-2006)
      5. Georgia Tsolou (2005-2011)
      6. Chunggi Baig (2006-2012)
      7. Orestis Alexiadis (2009-2014)
      8. Dimitris Tsalikis (2011 - to date)
      9. Katerina Karadima (2013 - to date)
      10. Stavros Peroukidis (2017 - to date)
      11. Terpsichori Alexiou (2017 - to date)

**STUDENT ADVISEMENT, ETH-ZURICH, PARTICLE TECHNOLOGY LABORATORY, DEPARTMENT OF MECHANICAL AND PROCESS ENGINEERING**

### Diploma Thesis students

1. Saskia Kohler (academic advisor: Prof. S.E. Pratsinis, graduated in 2015)
2. Natalia Smatsi (academic advisor: Prof. S.E. Pratsinis, graduated in 2018)
3. Simon Benz (academic advisor: Prof. S.E. Pratsinis, graduated in 2019)

### Masters’ Degree students

1. Vasil Vasilev (academic advisor: Prof. S.E. Pratsinis, graduated in 2017)
2. Natalia Smatsi (academic advisor: Prof. S.E. Pratsinis, Sept. 2017-to date)

### Ph.D. students

1. Anastasia Spyrogianni (academic advisor: Prof. S.E. Pratsinis, graduated in 2017)
2. Alexander Weyman (academic advisor: Prof. H.C. Öttinger, 2017-to date)

### Post-Doctoral Collaborators

1. Nikolaos Lempesis (2017-2018)

# REVIEWER FOR SCIENTIFIC JOURNALS

Reviewer for manuscripts submitted for consideration for publication in:

* *ACS Applied Nano Materials*
* *ACS Macro Letters*
* *ACS Nano Letters*
* *Advanced Composite Letters*
* *AICHE Journal*
* *Cellulose*
* *Chemical Engineering Research and Design*
* *Chemical Engineering Science*
* *Computational Materials Science*
* *Computers & Chemical Engineers*
* *Computer Physics Communications*
* *European Polymer Journal*
* *Europhysics Letters*
* *Industrial & Engineering Chemistry Research*
* *Journal of Advanced Physics*
* *Journal of the American Chemical Society*
* *Journal of Applied Physics*
* *Journal of Chemical Physics*
* *Journal of Crystal Growth*
* *Journal of Fluid Mechanics*
* *Journal of Fluorine Chemistry*
* *Journal of Hazardous Materials*
* *Journal of Materials Chemistry C*
* *Journal of Membrane Science*
* *Journal of Molecular Modeling*
* *Journal of Nanostructured Polymers and Nanocomposites*
* *Journal of Non-Equilibrium Thermodynamics*
* *Journal of Non-Newtonian Fluid Mechanics*
* *Journal of Polymer Science, Part B: Polymer Physics*
* *Journal of Physical Chemistry A,B,C*
* *Journal of Rheology*
* *Journal of Supercritical Fluids*
* *Korea-Australia Rheology Journal*
* *Fluid Phase Equilibria*
* *Langmuir*
* *Macromolecules*
* *Macromolecular Rapid Communications*
* *Macromolecular Theory and Simulation*
* *Materials Chemistry and Physics*
* *Molecular Simulation*
* *Nano Letters*
* *New Journal of Physics*
* *Physica A*
* *Physical Chemistry Chemical Physics (PCCP)*
* *Physics Letters A*
* *Physical Review E*
* *Physical Review Fluids*
* *Physical Review Letters*
* *Physics of Fluids*
* *Polymer*
* *Reactive and Functional Polymers*
* *Rheologica Acta*
* *Royal Society Advances*
* *Scientific Reports*
* *Soft Matter*
* *Theoretical and Computational Polymer Science*

# REVIEWER FOR FUNDING ORGANIZATIONS

Reviewer for proposals submitted for consideration for funding in:

* *Dutch Polymer Institute (DPI, The Netherlands)*
* *National Science Foundation (NSF, USA)*
* *The Petroleum Research Fund (ACS-PRF, USA)*
* *Greek Secretariat For Research and Technology (GSRT, Greece)*
* *Greek Ministry of Education and Religious Affairs (Greece)*
* *Research Committee, National Technical University of Athens (NTUA, Greece)*

# ORGANIZATION OF SCIENTIFIC MEETINGS

1. Member, Organizing Committee, *2nd International Meeting of the Hellenic Society of Rheology*, Heraklion, Crete, Greece, August 31-September 1st, **1998**.
2. Chairman, Organizing Committee, *3rd International Meeting of the Hellenic Society of Rheology*, Patras, Greece, June 10-June 14, **2001** (Conference dedicated to Prof. Andreas Acrivos on the occasion of his retirement from the Levich Institute, The City College of the City University of New York).
3. Member, Scientific Committee, *5th Panhellenic Conference on Polymers*, Heraklion, Crete, Greece, December 15-17, **2001**.
4. Member, Organizing Committee, *4th Panhellenic Chemical Engineers’ Conference*, Patras, Greece, May 30-June 1, **2003**.
5. Member, Scientific Committee, *2nd International Workshop and Summer School of Nonequilibrium Thermodynamics and Complex Fluids,* Princeton, USA, August 14-17, **2003**.
6. Member, Organizing Committee, *3rd Annual European Rheology Conference (AERC-2006),* Crete, Greece, April 27-29 **2005.**
7. Chairman, Organizing and Scientific Committee, *4th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET),* Rhodes, Greece, September 4-7, **2006**.
8. Member, Organizing Committee, *11th International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD 2007)*, Crete, Greece, May 20-25, **2007**.
9. Vice-Chair, Organizing and Scientific Committee, *15th International Workshop of Numerical Methods for Non-Newtonian Flows,* Rhodes, Greece, June 14-17, **2007**.
10. Member, Scientific Committee, *4th International Conference from Scientific Computing to Computational Engineering(4th IC-SCCE),* Athens, Greece, July 7-10, **2010**.
11. Member, Organizing and Scientific Committee, *7th International Workshop on Non-equilibrium Thermodynamics and Complex Fluids (IWNET 2015),* Hilvarenbeek, The Netherlands, July 6-10, **2015**.
12. Member, Scientific Committee, *European Polymer Gongress (EPF 2019),* Heraklion, Crete, Greece, June 9-14, **2019**.
13. Member, Scientific Committee, *International Conference on Adhesion in Aqueous Media: From Biology to Synthetic Materials (AAM 2019)*, Hilton Dresden, Germany, September 9-12, **2019**.

## SERVICES TO THE DEPARTMENT OF CHEMICAL ENGINEERING

* + - 1. Seminars Committee
* Chairman: 2003-2005, 2005-2007
* Member: 2007-2009, 2009-2011, 2011-2013
  + - 1. Committee of Undergraduate Studies, Member, 2003-2005
* Member: 2003-2005, 2005-2007, 2007-2009, 2009-2011,2011-2014
  + - 1. Committee of Graduate Studies, Chairman, 2007-2009
* Member: 2005-2007
* Chairman: 2007-2009, 2009-2011, 2011-2014, 2017-2020
  + - 1. Committee of Research and Academic Development, Member, 2007-2009
* Member: 2005-2007, 2007-2009
  + - 1. Committee of Computing and Network Infrastructure
* Member: 2009-2011, 2011-2014
  + - 1. Department’s Internal Evaluation Committee
* Member: 2011-2014

**REFERENCES**

Prof. Antony N. Beris Prof. Doros Theodorou

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