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LANGUAGES

Fluent in English, Greek

LEISURE ACTIVITIES

Literature and poetry reading, byzantine music, athletics

PERSONAL

Date of birth: January 14, 1982
Family status: Married, one son
Citizenship: Cypriot

ACADEMIC INTERESTS

Physical Chemistry:	Equilibrium Thermodynamics, Statistical Thermodynamics, Non-Equilibrium Thermodynamics, Statistical Mechanics
Materials:	Fluid Mechanics, Dynamics of Polymeric Liquids, Polymer Rheology, Polymer Physics, Statistical Mechanics of Polymers, Polymer Mechanics, Nanomaterials
Numerical Analysis:	Numerical Methods for Engineers, Finite Element Method

RESEARCH INTERESTS

Polymers:	Modelling at the mesoscopic and macroscopic level, rheological and dynamical behaviour, interfacial properties
Thermodynamics:	Generalized Bracket formalism of Beris-Edwards, GENERIC formalism of Grmela-Öttinger
Numerical Analysis:	Calculation of the fluxes of polymeric liquids using the Finite Element method

EDUCATION

Ph.D. and MSc in Chemical Engineering
Department of Chemical Engineering (DCE), University of Patras (UP), Greece, December **2006** – May **2011**

- *GPA*: 9.75/10.0 (top of class)
- *Dissertation*: "Development of scale-bridging methodologies and algorithms founded on the

outcome of detailed atomistic simulations for the reliable prediction of the viscoelastic properties of polymer melts"

- *Advisor*: Prof. Vlasis G. Mavrantzas

Diploma in Chemical Engineering

Department of Chemical Engineering, University of Patras, Greece, September **2001** – December **2006**

- *GPA*: 9.27/10.00 (top of class, **Third Highest GPA ever**)
- *Diploma thesis*: "Atomistic modelling of the polyelectrolyte membrane Nafion®"
- *Advisor*: Prof. Vlasis G. Mavrantzas

EXPERIENCE

Post-Doctoral Researcher (Special Scientist) (September **2016** – Today)

Department of Mathematics and Statistics (DMAS), University of Cyprus (UCY), Cyprus (with Prof. G. Ch. Georgiou)

Research Outline

- Thermodynamically guided non-equilibrium simulations of entangled polymer melts (with Profs. H. C. Öttinger and M. Kröger, Department of Materials (DMAT), ETH-Zürich (ETH-Z), Institut für Polymere, Zürich, Switzerland)
- Solving modifications of the Curtiss-Bird model using Brownian Dynamics simulations (with Prof. M. Kröger, DMAT, ETH-Z, Institut für Polymere)
- Constitutive equations for entangled polymer melts and solutions guided by principles of non-equilibrium thermodynamics (with Prof. V.G. Mavrantzas, Laboratory of Statistical Thermodynamics and Macromolecules (LSTM), DCE, UP, Greece and Department of Mechanical Engineering (DME), ETH-Z)
- Derivation of a generalized constitutive model for blood based on principles of non-equilibrium thermodynamics (with Prof. A.N. Beris, Depart. of Chemical and Biomolecular Engineering (DCBE), University of Delaware (UDEL), DE, USA)
- Multi-scale modelling of polymer-based nanocomposites (with Prof. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z)

Post-Doctoral Research Assistant (March **2015** – September **2016**)

DMAT, ETH-Z, Institut für Polymere, Zürich, Switzerland (with Profs. H. C. Öttinger and M. Kröger)

Research Outline

- Thermodynamically guided non-equilibrium simulations of entangled polymer melts
- Solution of the Curtiss-Bird model using Brownian Dynamics simulations
- Constitutive equations for entangled polymer melts and solutions guided by principles of non-equilibrium thermodynamics (with Prof. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z)
- Study of the settling of fractal-shaped agglomerates via Brownian Dynamic simulations (with Prof. S.E. Pratsinis, DME, ETH-Z)
- Derivation of a generalized constitutive model for blood based on principles of non-equilibrium thermodynamics (with Prof. A.N. Beris, DCBE, UDEL, DE, USA)

Post-Doctoral Researcher (Special Scientist) (August **2011** – February **2015**)

DMAS, UCY, Cyprus (with Prof. G. Ch. Georgiou)

Research Outline

- Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics.
- Multi-scale modelling (coupling MD simulations with a PP analysis and using elements of the reptation theory) aiming to predict the key material properties of higher-MW polymers starting from a detailed analysis of the dynamic properties of considerably shorter (but entangled) samples (with Prof. V.G. Mavrantzas, DCE, UP, Greece)

Ph.D. Research Assistant (September **2008** – April **2009**)
Department of Chemical and Biomolecular Engineering, The University of Tennessee-Knoxville, TN, USA (with Profs. B. J. Edwards and B. Khomami)

Research Outline

- Development of Brownian Dynamics algorithms for bead-spring chains with anisotropic friction tensors
- Comparing their predictions with non-equilibrium atomistic molecular dynamics (NEMD) simulations of unentangled polymer melts

Ph.D. Research Assistant (September **2006** – May **2011**)
LSTM, DCE, UP, Greece (with Prof. V. G. Mavrantzas)

Ph.D. Thesis Research Outline

- Development of a Generalized Hamiltonian model (based on the Generalized Bracket Formalism of Beris-Edwards) for the description of the rheology of unentangled polymer melts and solutions.
- Derivation and solution of the Rouse model for ring polymers
- Detailed comparison of the predictions of the Doi-Edwards reptation theory and modern tube models for entangled polymers melts with the results of detailed atomistic molecular dynamics simulations for model monodisperse and bidisperse systems of polyethylene and polybutadiene.

Classes

- Attended 7 postgraduate classes in the Department of Chemical Engineering: "Applied Mathematics", "Advanced Thermodynamics", "Advanced Numerical Methods" (Finite Elements Method), "Advanced Transport Phenomena", "Polymer Rheology", "Dynamical Systems", "Advanced Statistical Mechanics", "Molecular Simulation Theory"
- Attended classes in other Departments and Graduate Programs of the University of Patras, Greece: Inter-Departmental Program "Polymer Science and Technology" ("Polymer Physics", "Polymer Physical Chemistry"), Mathematics Department ("Stochastic Processes", "Stochastic Analysis"), Physics Department ("Statistical Physics").

Projects during undergraduate and graduate courses

- "Determination of the thermodynamic functions of H_2WO_4", Project undertaken during "Physical Chemistry II" course, May **2003**.
- "Estimation of the second virial coefficient, the compressibility factor and the fugacity coefficient for N_2, O_2, Ar, Xe, and CO_2", Project report independently prepared, February **2005**.
- "Estimation of the second virial coefficient, the compressibility factor and the fugacity coefficient for H_2, CH_4, ethane, ethene, ethyne, propane and i-butane", Project report independently prepared, February **2005**.
- "The organizational structure of Nafion: The integral equation theory", Project undertaken during "Special Chapters of Physical Chemistry" course, November **2005**.
- "Phase Equilibrium and Stability in mixtures using non-linear programming", Project undertaken during "Process Optimization" course, June **2006**.
- "Utilizing a new hybrid model for simulating the filament stretching experiment" with A. Anastasiou, Project undertaken during "Advanced Numerical Methods" course, Fall **2008**.

TEACHING

Undergraduate Courses

- "Mathematics II" MEM_102, Department of Mechanical Engineering and Materials Science and Engineering (DMEMSE), Cyprus University of Technology (CUT), Spring **2017**.
- "Numerical Methods in Engineering" MEM_329, DMEMSE, CUT, Fall **2017**.

Teaching Assistant

- "Physical Chemistry II" (DCE/UP, Prof. V.G. Mavrantzas: Spring **2007**, Spring **2008**, Spring **2010**)
- "Polymer Science" (DCE/UP, Prof. C. Tsitsilianis: Fall **2007**)
- "Polymer Rheology" (DCE/UP, Prof. V.G. Mavrantzas: Fall **2009**, Fall **2010**)
- "Transport Phenomena I" (DMAT\ETH-Z, Prof. H.C. Öttinger, Fall **2015**).
- "Transport Phenomena II" (DMAT\ETH-Z, Prof. H.C. Öttinger, Spring **2016**).

Teaching Replacement

- "Engineering Mathematics II", MAS026 (DMAS\UCY, Prof. G. Ch. Georgiou, Fall **2016**)
- "Fluid Mechanics", MAS483 (DMAS\UCY, Prof. G. Ch. Georgiou, Spring **2017**)

Informal Teaching

Taught (in weekly group meetings in **2006**) with Dr. Chunggi Baig (now Assistant Professor, Ulsan National Institute of Science and Technology (UNIST), South Korea) the following textbooks:

- "Beyond equilibrium thermodynamics" by H.C. Öttinger.
- "Theory of Polymer Dynamics" by M. Doi and S.F. Edwards.

MILITARY SERVICE (COMPULSORY IN CYPRUS)

- Cyprus National Guard, Nicosia, Cyprus (July **1999** – September **2001**)

HONORS AND AWARDS

- Top of Class Award for Undergraduate studies, State Scholarship Foundation, annually **2001** – **2006**.
- Top of Class Award for Undergraduate studies for the academic year 2003-2004, Technical Chamber of Greece, **2007**.
- Top of Class Award for excellence in Undergraduate studies, Technical Chamber of Greece, **2008**.
- Swiss Government Excellence Scholarship for Foreign Scholars, 09/**2015**–08/**2016** (ESKAS No. 2015.0297).
- Cyprus Research Award – "Young Researcher" 2015 (Thematic Area: Physical Sciences and Engineering), November **2015**, https://www.youtube.com/watch?v=SX1OC-xs9zA (in Greek).
- Marie Sklodowska-Curie Actions Seal of Excellence, 25/04/**2017** (this quality label is awarded to all proposals submitted to the MSCA Individual Fellowships Call that scored 85% or more but could not be funded from the call budget; for the year 2017 the seal was awarded to 2300 researchers on a Pan-European level)

PROFESSIONAL AFFILIATIONS

- Member, Hellenic Society of Rheology (HSR)
- Member, European Society of Rheology (ESR)
- Member, Society of Rheology (SOR)
- Member, American Chemical Society (ACS)

PARTICIPATION IN RESEARCH AND DEVELOPMENT PROJECTS

Karatheodori 2004

- 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 k€
- Contribution to the LSTM Lab: 23.5 k€
- Duration: **2004** – **2007**
- Project coordinator: V.G. Mavrantzas

DOW Chemicals Industrial project II

- 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 k€
- Contribution to the LSTM Lab: 75 k€
- Duration: **2006** – **2008**
- Project coordinator: V.G. Mavrantzas

PolyHub

- National Science Foundation grant
- Contract No: CBET-0742679
- Partners: University of Tennessee-Knoxville (UTK) (Coordinator), Max Planck Institute of Polymer Research (MPIPR), Stanford University (US), ETH-Z, University of Patras (UP), and Illinoi Institute of Technology (IIT).
- Total budget: 190 k$
- Duration: **2007** – **2009**
- Project coordinator: B. J. Edwards

MODIFY

- EC (FP7-NMP-2008-SMALL-2) project titled: *Multi-scale modeling of interfacial phenomena in acrylic adhesives undergoing deformation*
- Funding Body: EU
- Contract No: 228320
- Partners: Univ. of Patras (Coordinator), Ecole supérieure de physique et de chimie industrielles de la ville de Paris (ESPCI ParisTech), Centre national de la recherche scientifique (CNRS), University College London (UCL), ETH-Z, Dow Chemical Company, LBI.
- Total EC contribution: 2,863 k€
- EC contribution to the LSTM Lab: 402.3 k€
- Duration: **2009** – **2012**
- Project coordinator: V.G. Mavrantzas

VISCOnanoNET

- Marie Curie Reintegration grant titled: *Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics*
- Funding Body: EU
- Contract No: FP7-PEOPLE-2011-CIG, Code 293945
- Partners: Univ. Cyprus (Coordinator), Univ. Patras
- EC contribution: 75 k€
- Duration: 08/**2011** – 06/**2012** [Terminated as it was not possible to have it funded simultaneously with ΔΙΔΑΚΤΩΡ/0311/40]
- Project coordinator: G.C. Georgiou

VISCOnanoNET

- National grant titled: *Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics*
- Funding Body: Cyprus Research Promotion Foundation
- Contract No: ΔΙΔΑΚΤΩΡ/0311/40
- Partners: Univ. Cyprus (coordinator), Univ. Patras
- EC contribution: ~106 k€

- Duration: 07/**2012** – 12/**2014**
- Project coordinator: G.C. Georgiou

MultiScalePNC

- National grant titled: *Multiscale modelling of polymer nanocomposites*
- Funding Body: Cyprus Research Promotion Foundation (RPF); made available through the Cyprus Research Award - "Young Researcher" 2015.
- Contract No: ΚΟΥΛΤΟΥΡΑ/ΒΡ-ΝΕ/0415/01
- Partners: Univ. Cyprus
- RPF contribution: 35 k€
- Duration: 09/**2016** – 04/**2018**
- Project coordinator: P.S. Stephanou

RESEARCH ACTIVITIES

A major theme of my research work has been the development of reliable constitutive models for describing the dynamics and flow behavior of complex polymeric fluids. To this, I rely on the use of non-equilibrium thermodynamics (NET), in particular on the Generalized Bracket and GENERIC formalisms, for developing closed-form balance equations for the fundamental hydrodynamic fields. **No matter what the system is (say biological or chemical), it must obey the laws of thermodynamics.** In particular, when the system is beyond equilibrium (e.g., under the influence of a flow field), its time evolution must be dictated by the laws of non-equilibrium thermodynamics (NET). This is exactly the reason for employing NET in my work: by construction the new constitutive models obey the laws of thermodynamics. In my models, the underlying microstructure of the complex fluid is described by using structural variables, such as the conformation tensor for polymer chains (describing their average conformation), which are hydrodynamically coupled with the imposed flow field. The relation between microstructure (structural variables) and macroscopic observables (viscometric functions) takes eventually the form of a stress tensor equation. **So far, I have developed generalized constitutive models for polymer melts, polymer solutions, and polymer nanocomposites**. **Currently, I am using NET to develop constitutive models for biomolecular fluids, such as blood.**

In most cases, the resulting constitutive equations contain parameters whose values are not known. To overcome this, I resort to atomistic simulations, both (equilibrium) Molecular Dynamics (MD) and non-equilibrium MD (NEMD). This allows me to develop interconnections between three different levels of system description: the atomistic or microscopic, the mesoscopic, and the macroscopic. As one moves from the atomistic to the macroscopic level (coarse-graining), the degrees of freedom of the system are significantly reduced, which results in a dramatic reduction in computational demands. However, coarse-graining must be done carefully to avoid the loss of important information. My work connects the three levels through the development of scale-bridging methodologies, and the outcome is a set of, closed-form, constitutive equations for the time evolution of the structural and hydrodynamic fields selected to describe the system. Overall, the building blocks of my bridging methodology are the following:

1) At the **atomistic level**: I use atomistic MD and NEMD simulations to simulate the real system and obtain the values of important parameters entering the description of the system at the mesoscopic level.
2) At the **mesoscopic level**: I design coarse-grained simulations (e.g. Brownian dynamics (BD) simulations, Dissipative Particle Dynamics (DPD), coarse grained MD) which provide information about the evolution of the system for much larger time spans than what is addressed by atomistic simulations.
3) At the **macroscopic level**: I use NET to derive generalized constitutive models for complex systems whose parameters are evaluated from the previous levels.

MAJOR PROBLEMS ADDRESSED

1) Constitutive equations for unentangled polymer melts guided by principles of non-equilibrium

thermodynamics **[Ref.: 1]**

Based on principles of non-equilibrium thermodynamics, we derived a generalized constitutive model 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 (one evolution equation for the conformation tensor and one relating the stress tensor with the conformation tensor), 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 model are the functions describing the dependence of the non-equilibrium free energy and relaxation matrix on the conformation tensor. Restrictions on the parameters entering these two functions have been obtained by analyzing the thermodynamic admissibility of the model. With suitable choices of these two functions, the new set of equations reduces to many well-known viscoelastic models. The new equations are used to describe (fit) rheological data provided either by experimental measurements on industrial samples [P. S. Stephanou, C. Baig, V.G. Mavrantzas, and J. Den Doelder, (2011) (report)] or obtained through Non-Equilibrium Molecular Dynamics (NEMD) simulations in shear and planar elongation.

2) Topological and dynamical mapping of atomistic simulation results onto the tube model of the reptation theory for the dynamics of entangled polymers **[Refs.: 2,3,5,7-10]**

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 the way to interfacing atomistic simulation data with reptation, admittedly the most successful phenomenological theory of polymer dynamics for entangled systems. We have developed 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 $\psi(s,t)$, namely the probability that a segment s of the primitive chain remains inside the initial tube after time t. We have utilized this information 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 have gained a deeper understanding of the predominant relaxation mechanisms in entangled polymers, and thus succeeded in our effort to encode this information in the form of suitable (more accurate) constitutive equations.

3) Rouse Theory for cyclic polymeric chains (rings) **[Ref.: 4]**

We have presented a comprehensive analysis of the full Rouse theory for rings, together with a complete appreciation of its predictions for a variety of rheological properties. Although, researchers have previously presented several of these predictions, here we present the theory to its entirety for both the continuous and discrete model. Our analysis refers to a melt composed of short unentangled ring molecules, where hydrodynamic interactions are assumed to be effectively screened out and no topological interactions between molecules need to be considered. The Rouse theory is found to provide a satisfactory description of recent atomistic simulation findings (of strictly monodisperse model unentangled ring polyethylene (PE) melts ranging in chain length from C24 up to C400 at temperature T=450 K and P=1 atm, especially for rings with chain length between C50 and C170. An important finding of these simulations (from the observed dependence of the chain center-of-mass self-diffusion coefficient, D_G, the characteristic spectrum of the Rouse relaxation times, τ_p, the monomeric friction coefficient, ζ, and the zero-shear rate viscosity, η_0, on chain length N) is that PE ring melts follow approximately Rouse-like dynamics even when their chain length is as long as C400; this is more than twice the characteristic crossover chain length (~C156) marking the passage from Rouse to reptation dynamics for the corresponding linear PE melts).

4) BD simulations of unentangled polymeric liquids and semi-dilute solutions **[Ref.: 6]**

We have presented BD simulations of unentangled polymeric materials under shear flow, with polymer molecules modelled as bead-spring chains using the finitely extensible nonlinear elastic (FENE) force law. The reptation idea (that a chain diffuses in an entangled melt more easily in the direction parallel to its molecular axis than perpendicular to it) was also implemented in these simulations; it was incorporated in a mean-field approach through an anisotropic diffusion matrix representing enhanced diffusion along the chain background once chains have been significantly extended or oriented in response to the applied flow field. The predictions of the BD simulations, with only one single adjustable parameter (the degree of relative diffusive enhancement along the chain backbone), were in remarkable quantitative agreement with atomistic NEMD simulation data of short-chain polyethylene liquids and experimental results for semi-dilute DNA solutions under shear. The model underlying the BD simulations was further coarse-grained to the continuum level through pre-averaging, and its predictions served to examine the relationship between two different levels of description; the continuum model matched the mesoscopic model at low shear rates, but greatly diverged at high shear rates where the tumbling dynamics of the individual chains dominated the system response. A significant conclusion from this work was that the onset of rotational motion under shear is responsible for the well-known breakdown in pre-averaged constitutive equations at the continuum level of description.

5) Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics **[Refs.: 11,12]**

By appropriately adding nanoparticles to a polymer matrix can lead to materials with dramatically improved properties, especially under conditions of good dispersion. From a rheological point of view, polymer nanocomposites are typically considered to be soft colloidal dispersions, with an intrinsically disordered structure that greatly affects their viscoelastic or mechanical properties. Despite that the rheological properties of nanocomposites in the melt can be predicted or explained via entanglement network simulations based on multi-scale simulation strategies, large-scale macroscopic calculations of their processing flows require reliable constitutive (viscoelastic) equations which are currently missing.

In the present research activity, the Generalized Bracket framework has been extended to handle mixed systems consisting of two phases: a polymer matrix and a dispersed phase of spherical nanoparticles. The proposed work is, to the best of our knowledge, one of the very first efforts undertaken world-wide to describe the mechanical-rheological response of these materials through thermodynamically admissible, closed-form constitutive expressions. For the polymer component, we have used the general viscoelastic model for homopolymer melts, of which the structural variable is the conformation tensor $\boldsymbol{C}$, accounting for several complex phenomena and interactions proposed recently by Stephanou et al. [Ref. 1]. To account for the nanoparticles, we employ the orientation tensor $\boldsymbol{a}$ which attains a constant trace. This continuum model can describe in a unified and self-consistent way the microstructure, phase behavior, and rheology in both the linear and non-linear regimes of polymer nanocomposites. The dynamic equations are developed for nanoparticles with an arbitrary shape but then they are specified to the case of spherical ones. Restrictions on the parameters of the model are provided by analyzing its thermodynamic admissibility. A key ingredient of the model is the expression for the Helmholtz free energy A of the polymer nanocomposite. At equilibrium, this reduces to the form introduced by Mackay et al. to explain the phase behavior of polystyrene melts filled with silica nanoparticles. Beyond equilibrium, A contains additional terms that account for the coupling between microstructure and flow. In the absence of chain elasticity, the proposed evolution equations capture known models for the hydrodynamics of a Newtonian suspension of particles. A thorough comparison against several sets of experimental and simulation data demonstrates the unique capability of the model to accurately describe chain conformation and swelling in polymer melt nanocomposites, and to reliably fit measured rheological data for their shear and complex viscosity over large ranges of volume fractions and deformation rates. We also address the issue of flow effects on the phase behavior of polymer nanocomposite melts. For this purpose, we calculate the spinodal curve, by computing values for the nanoparticle radius as a function of the polymer radius-of-gyration for which the second derivative of the generalized free energy of the system with respect to the volume fraction becomes zero. Under equilibrium conditions, we recover the phase diagram predicted by Mackay et al. Overall, our model

predicts that flow enhances miscibility, since the corresponding miscibility window opens up for non-zero shear rate values. To the best of our knowledge, this is the first theoretical study which addresses this problem and produces results in accord with experimental findings, especially for the phase behavior. These theoretical results provide new insights into understanding the interrelation of nanostructure, phase behavior (miscibility) and rheology. This research project received the «Cyprus Research Award–Young Researcher 2015» (Thematic area: Physical Sciences and Engineering) in the context of which the Dr. Stephanou has received a research grant (equal to 35 kEuros) from the Research Promotion Foundation (RPF) of Cyprus. Website: http://euclid.mas.ucy.ac.cy/~visconan/

Overall, the applications of NET cover a wide range of problems in the field of complex microstructured fluids (polymeric liquids, dispersions, emulsions, liquid crystals, adhesives, biological systems, etc.). In all these systems, adhering to a fundamental and strict NET framework is a prerequisite if one wishes to establish self-consistent links between different levels of description (each level addressing phenomena over a specific window of length and time scales) related to structure/morphology development, relaxation, and deformation. In our future undertakings, we aim to use both NET and (atomistic and coarse-grained) simulations to study currently open and fascinating problems in the field of complex microstructured fluids:

CURRENT RESEACH-BRIEF OUTLINE

6) Constitutive equations for Entangled polymer melts and solutions guided by principles of non-equilibrium thermodynamics **[Refs.: 13,18]**

Our aim is to provide a description of the Marrucci−Ianniruberto constitutive equation for the rheology of entangled polymer melts in the context of non-equilibrium thermodynamics and we properly extend it to account for a second normal stress difference by introducing a second order term in the relaxation tensor in terms of the conformation tensor. The modified model incorporates one additional parameter, the anisotropic mobility parameter α, which allows for a non-vanishing prediction of the second normal stress coefficient, but still considers a constant entanglement density. Application of the second law of thermodynamics and the requirement that the evolution equation must preserve the positive-definite nature of the conformation tensor between successive entanglement points along the chain for all times and all flow fields constrain the convective constraint release (CCR) parameter β_{ccr} to values strictly greater than one ($\beta_{ccr}>1$) and the new parameter α to values in the interval $0\leq\alpha\leq1-\beta_{ccr}^{-1}$. The modified model provides a satisfactory description of available experimental data for the transient and steady-state shear rheology of entangled polystyrene melts and for the elongational steady-state stress of an entangled polystyrene solution over the entire range of shear and elongation rates covered in the rheological measurements. Current efforts are focused on extending this model so as it allows for a decreasing entanglement density.

7) Solution of the complete Curtiss-Bird model using BD simulations **[Refs.: 14-17]**

We solve the complete Curtiss-Bird model (that we coin the tumbling-snake model), a kinetic theory for concentrated polymer melts and concentrated solution. This model has only been solved for the special case in which one of its parameters, ε', is set to 0, termed the simplified Curtiss-Bird model. The importance of solving the complete model is exemplified by the fact that the power-law behavior at high shear rates is very different for when $\varepsilon'=0$ and when $\varepsilon'=1$, in which case the whole chain behaves as a Brownian rod-like polymer; thus the intermediate cases, $0<\varepsilon'<1$, may be of relevance for (i) the modelling of concentrated solutions or melts of semi-flexible polymers, and (ii) a better description of experimental data including power-law behavior at accessible rates that is intermediate between the known asymptotic behaviors of rod-like and fully flexible systems. The model has been favorably compared with available rheological data for semi-flexible biological systems that are clearly not captured by the simplified Curtiss-Bird model for steady-state shear flow. We have further shown that the tumbling-snake model is able to quantitatively capture the damping behavior (the appearance of an undershoot following the overshoot) in the transient shear viscosity of a concentrated polymeric solution, supplemented by a non-constant link-tension coefficient that we relate to the nematic order parameter. The observed phenomena are attributed to the tumbling behavior of the links, triggered by rotational fluctuations, on top of reptation. Overall, the tumbling-snake model has the promising

capacity to improve our understanding of the transient behavior of concentrated polymer Currently, the complete model is solved, again via BD simulations, for both transient and steady-state elongation flows.

8) Multi-scale modeling of polymer nanocomposites **[Refs.: 19,20]**
Using the results of detailed atomistic non-equilibrium molecular dynamics (NEMD) simulations we calculate the values of the parameters found in a recently proposed constitutive model for polymer nanocomposites (PNCs). We shall also extend a recently proposed model for entangled polymer melts and solutions [Refs. 13,18] to the intriguing case of entangled PNCs. It has been noted that PNCs with spherical NPs in which the matrix is entangled (entangled PNCs) exhibit a *decreasing* zero-shear-rate viscosity at small nanoparticle volume fractions, which clearly comes at odds with Einstein's theory. We will also perform atomistic NEMD simulations for both polymer melts and PNCs and extract the values of the parameters needed in the constitutive equations (the macroscopic level).

9) Studying the rheological behavior of blood **[Ref.: 21]**
Based on principles of non-equilibrium thermodynamics, we derive a generalized constitutive model for blood. In particular, we are re-deriving the constitutive model of Owens (which accounts for the complicated dynamical formation of rouleaux) from a NET perspective and properly generalize it.

10) Modelling the viscoelasticity of Newtonian nanocomposites guided by principles of non-equilibrium thermodynamics **[Refs.: 22,23]**
Based on principles of non-equilibrium thermodynamics, we derive a generalized constitutive model for Newtonian nanocomposites with non-spherical fillers.

11) Thermodynamically Guided non-equilibrium simulations of Entangled polymer melts **[Ref.: 24]**
We wish to obtain the dissipative component in the GENERIC modelling of entangled polymer melts directly from coarse-grained MD and Monte-Carlo simulations.

12) Flow behavior of nanoparticles in blood (theory, coarse-grained simulations, and finite-element calculations)
The injection of drug-carrying NPs in blood is increasingly becoming a reality. One of our future tasks is to provide the NET description and flow behavior of NPs in blood vessels and capillaries. Coarse-grained simulations (e.g. DPD simulations) of NPs in blood will also be conducted.

13) Turbulence from a NET perspective (theory and numerical analysis)
We wish to use NET, and in particular GENERIC, in order to model irreversible energy cascade in turbulence from larger down to smaller scales without entropy production by building on the recent work of Öttinger. In a later stage, we will derive the corresponding equations for the turbulent flow of complex fluids; this will allow us to study a plethora of important research questions: the polymer-induced drag reduction and the turbulent flow of agglomerated NPs at very high Reynolds numbers (with tremendous applications in the field of aerosols and in atmospheric pollution).

14) Theory of the complex conservation phenomenon
We wish to use NET to study the complex conservation phenomenon, appearing when a polycation and a polyanion are mixed under proper pH conditions

PUBLICATIONS IN REFEREED JOURNALS (* denotes corresponding author)

1. **P. S. Stephanou**, C. Baig, V.G. Mavrantzas*, "A generalized differential constitutive equation based on principles of non-equilibrium thermodynamics", *J. Rheol.* 53, 309-337 **(2009)**. [Citations: 20]
2. **P. S. Stephanou,** C. Baig, G. Tsolou and V. G. Mavrantzas* and M. Kröger, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *J. Chem. Phys.* 132, 124904 **(2010)**. [Citations: 62]
3. C. Baig*, **P. S. Stephanou**, G. Tsolou, V. G. Mavrantzas and M. Kröger, "Understanding dynamics in binary mixtures of entangled cis-1,4-polybutadiene melts at the level of primitive path segments by mapping atomistic simulation data onto the tube model", *Macromolecules* 43,

8239-8250 **(2010)**. [Citations: 16]

4. G. Tsolou, N. Stratikis, C. Baig*, **P. S. Stephanou** and V. G. Mavrantzas*, "Melt Structure and Dynamics of Unentangled Polyethylene Rings: Rouse Theory, Atomistic Molecular Dynamics Simulation, and Comparison with the Linear Analogues", *Macromolecules* 43, 10692–10713 **(2010)**. [Citations: 43]
5. **P. S. Stephanou,** C. Baig* and V. G. Mavrantzas*, "Projection of atomistic simulation data for the dynamics of entangled polymers onto the tube theory: Calculation of the segment survival probability function and comparison with modern tube models", *Soft Matter* 7, 380–395 **(2011)**. [Citations: 21]
6. J. M. Kim, **P. S. Stephanou**, B. J. Edwards* and B. Khomami, "A mean-field anisotropic diffusion model for unentangled polymeric liquids and semi-dilute solutions: Model development and comparison with experimental and simulation data", *J. Non- Newtonian Fluid Mech.* 166, 593–606 **(2011)**. [Citations: 6]
7. **P. S. Stephanou**, C. Baig*, V.G. Mavrantzas*, "Toward an Improved Description of Constraint Release and Contour Length Fluctuations in Tube Models for Entangled Polymer Melts Guided by Atomistic Simulations", *Macromol. Theor. Simul*. 20, 752–768 **(2011)**. [Citations: 9]
8. J. Qin*, S. T. Milner, **P. S. Stephanou**, V.G. Mavrantzas, "Effects of Tube Persistence Length on Dynamics of Mildly Entangled Polymers", *J. Rheol.* 56, 707-723 **(2012).** [Citations: 10] *selected for the May 15, 2012 issue of Virtual Journal of Biological Physics Research (www.vjbio.org).*
9. **P. S. Stephanou***, V.G. Mavrantzas*, "Quantitative predictions of the linear viscoelastic properties of entangled polyethylene and polybutadiene melts via modified versions of modern tube models on the basis of atomistic simulation data", *J. Non- Newtonian Fluid Mech*. 200, 111-130 **(2013).** [Citations: 5]
10. **P. S. Stephanou***, V.G. Mavrantzas*, "Accurate prediction of the linear viscoelastic properties of highly entangled mono and bidisperse polymer melts", *J. Chem. Phys*. 140, 214903 (**2014**). [Citations: 5]
11. **P. S. Stephanou***, V.G. Mavrantzas, G. C. Georgiou, "Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts", *Macromolecules* 47,4493–4513 (**2014**). [Citations: 7]
12. **P. S. Stephanou***, "How the flow affects the phase behaviour and microstructure of polymer nanocomposites", *J. Chem. Phys.* 142, 064901 (**2015**). [Citations: 6]
13. **P. S. Stephanou***, I. Tsimouri, and V. G. Mavrantzas, "Flow-induced orientation and stretching of entangled polymers in the framework of non-equilibrium thermodynamics", *Macromolecules* 49, 3161–3173 (**2016**). [Citations: 1]
14. **P. S. Stephanou***, and M. Kröger, "Solution of the complete Curtiss-Bird model for polymeric liquids subjected to simple shear flow", *J. Chem. Phys*. 144, 124905 (**2016**). [Citations: 2]
15. **P. S. Stephanou***, T. Schweizer, and M. Kröger, "Communication: Appearance of undershoots in start-up shear: Experimental findings captured by tumbling-snake dynamics", *J. Chem. Phys*. 146, 161101 (**2017**). [Citations: 0]
16. **P. S. Stephanou***, and M. Kröger, "Non-constant link tension coefficient in the tumbling-snake model subjected to simple shear", *J. Chem. Phys.* 147 accepted (**2017**). [Citations: 0]

PUBLICATIONS SUBMITTED OR UNDER PREPARATION (* denotes corresponding author)

17. **P. S. Stephanou***, "The rheology of drilling fluids from a non-equilibrium thermodynamics perspective", *J. Pet. Sci. Eng.* submitted (**2017**).
18. **P. S. Stephanou***, and M. Kröger, "Solution of the complete Curtiss-Bird model for polymeric liquids subjected to uniaxial elongation", *J. Chem. Phys*. submitted (**2017**).
19. I. Ch. Tsimouri, **P. S. Stephanou**, and V. G. Mavrantzas, "A rheological model for blood from nonequilibrium thermodynamics: Model development", *Phys. Fluids*, to be submitted (**2017**).
20. **P. S. Stephanou**, I. Tsimouri, C. Georgakopoulos, and V. G. Mavrantzas, "Flow-induced orientation and stretching of entangled polymers in the framework of non-equilibrium thermodynamics: A revision", *Macromolecules* under preparation (**2017**).
21. **P. S. Stephanou**, and V.G. Mavrantzas, "Continuum Model for the Phase Behavior, Microstructure, and Rheology of Entangled Polymer Nanocomposite Melts", *Macromolecules*

under preparation (**201**7).

22. P. Alatas, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas, "Multiscale modeling approach to the rheological behavior of polymer nanocomposites: Nonequilibrum thermodynamics modeling coupled with NEMD simulations", *Macromolecules* under preparation (**2017**).
23. **P. S. Stephanou**, "Constitutive modelling of nanofiber suspensions", *J. Non-Newton. Fluid Mech.* under preparation (**2017**).
24. **P. S. Stephanou**, "A rheological description of nanoclay suspensions", *Rheol. Acta* under preparation (**2017**).
25. **P. S. Stephanou**, P. Ilg, H. C. Öttinger, and M. Kröger, "Thermodynamically Guided nonequilibrium simulations of entangled polymer melt", *Phys. Rev. E* under preparation (**2017**).

CITATIONS (until November 2017, based on Scopus database)
By others: 166
Self-citations: 47
Total: 213
Hirsch h index: 7

PUBLICATIONS IN CONFERENCE PROCEEDINGS

1. **P. S. Stephanou**, C. Baig, V.G. Mavrantzas, "Generalization of the Giesekus viscoelastic model and validation of its rheological predictions for polymer melts", Proceedings, *6th Panhellenic Chemical Engineers' Conference*, Vol. 2, p. 1065-1068, Athens, Greece, May 31-June 2 **(2007)**
2. **P. S. Stephanou**, C. Baig, G. Tsolou, V. G. Mavrantzas and M. Kröger, "Topological and Dynamical Mapping of Atomistic Simulation Data onto the Tube Model for Entangled Polymer Melts", CD version, *7th Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 3-5 **(2009).**
3. **P. S. Stephanou**, C. Baig, G. Tsolou and V. G. Mavrantzas, "Mapping atomistic simulation results for the dynamics of entangled polymer melts onto the tube model of the reptation theory", 4*th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE)*, p. 370-376, Athens, Greece, July 7-10 **(2010)**.
4. C. Baig, **P. S. Stephanou**, G. Tsolou, V. G. Mavrantzas and M. Kröger, "Mapping of atomistic simulation data for the dynamics of entangled polymers onto the tube model: Calculation of the segmental survival probability function for mono- and bi- disperse melts and comparison with modern tube models", Code 83459, *2010 AIChE Annual Meeting (10th AIChE)*, Salt Lake City, Utah; United States, November 7-12 **(2010)**.
5. G. Tsolou, N. Stratikis, **P. S. Stephanou**, C. Baig, and V. G. Mavrantzas, "Detailed Molecular-Dynamics Study On Structural and Dynamical Properties of Unentangled Ring Polyethylene Melts: Comprehensive Analysis of the Rouse Theory and Simulation", *2010 AIChE Annual Meeting (10th AIChE)*, Salt Lake City, Utah; United States, November 7-12 **(2010)**.
6. **P.S. Stephanou**, C. Baig, V.G. Mavrantzas, "Generalized viscoelastic model for polymer melts guided by principles of non-equilibrium thermodynamics: Single- and multi-mode formulations", *7th GRACM International Congress on Computational Mechanics*, Athens, Greece, June 30-July 2 **(2011).**
7. J. Qin, S. Milner, **P. S. Stephanou**, V. G. Mavrantzas, "Tube Dynamics of Mildly Entangled Polymers: Semiflexibility Effects", *APS Meeting Abstracts, Vol. 2, p. 49005* **(2012).**
8. **P. S. Stephanou** and V. G. Mavrantzas, "Multi-scale modelling of polymer melt viscoelasticity: From atoms, to molecules, to primitive paths, to tube models", CD version, 9^{h} *Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 23-25 **(2013)** [in Greek].
9. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A generalized differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics", CD version, 9th *Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 23-25 **(2013)** [in Greek].
10. T. Koukoulas, D. Tsalikis**, P.S. Stephanou** and V.G. Mavrantzas, "Conformational dynamics and topological analysis for polymer rings via atomistic Molecular-Dynamics simulations and comparison with experimental data", *10th HSTAM 2013 International Congress on Mechanics,*

Chania, Crete, Greece, May 25-27 **(2013)**.

11. V. G. Mavrantzas, Th. Koukoulas, D. Tsalikis, **P.S. Stephanou**, "Atomic molecular dynamics simulations of the conformational dynamic and topological properties of ring polymer melts", *Abstracts of papers of the American Chemical Society, Vol. 245* **(2013)**.
12. C. K. Georgantopoulos, I. Ch. Tsimouri**, P. S. Stephanou**, and V. G. Mavrantzas, "Derivation of modern rheological constitutive models through the use of non-equilibrium thermodynamics", *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
13. I. Ch. Tsimouri**, P. S. Stephanou**, and V. G. Mavrantzas, "A constitutive rheological model for blood through the use of non-equilibrium thermodynamics", *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
14. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Modelling polymer nanocomposites based on the principles of non-equilibrium thermodynamics modelling and the findings of detailed non-equilibrium atomistic simulations", *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
15. **P. S. Stephanou** and V. G. Mavrantzas, "Polymer melt viscoelasticity: from atomistic molecular dynamics simulations to the tube model", *11^{h} Panhellenic Chemical Engineers' Conference*, Thessaloniki, Greece, May 25-27 **(2017)**.
16. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Hierarchical modeling of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations", *Materials Today: Proceedings* **(2017).**

INVITED PRESENTATIONS (Speaker underlined)

1. **P. S. Stephanou**, D. G. Tsalikis, and V. G. Mavrantzas, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Non-equilibrium thermodynamics modelling coupled with NEMD simulations", *8th International Conference on Multiscale Materials Modelling,* Dijon, France, October 9-14 **(2016)**.

PRESENTATIONS IN CONFERENCES (Speaker underlined)

1. **P. S. Stephanou**, C. Baig, V. G. Mavrantzas, "Generalization of the Giesekus viscoelastic model and validation of its rheological predictions for polymer melts", Proceedings, *6st Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 31-June 2 (**2007).** [In Greek]
2. **P. S. Stephanou**, C. Baig, V.G. Mavrantzas, "A generalized single-conformation tensor viscoelastic model based on principles of non-equilibrium thermodynamics (poster)", *XVth International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2007),* Rhodes, Greece, June 6-10 **(2007)**.
3. **P. S. Stephanou**, C. Baig, G. Tsolou, V. G. Mavrantzas and M. Kröger, "Topological and Dynamical Mapping of Atomistic Simulation Data Onto the Tube Model for Entangled Polymer Melts", Proceedings, *7th Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 3-5 **(2009)**.
4. **P. S. Stephanou**, C. Baig, G. Tsolou and V. G. Mavrantzas, "Mapping atomistic simulation results for the dynamics of entangled polymer melts onto the tube model of the reptation theory", Proceedings, *4th International Conference from Scientific Computing to Computational Engineering (4th IC-SCCE),* Athens, Greece, July 7-10 **(2010)**.
5. **P.S. Stephanou**, G. Tsolou, N. Stratikis, C. Baig, V.G. Mavrantzas, "Rouse theory for polymer rings and comparison with atomistic molecular-dynamics simulations", *6th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 26-28 **(2011).**
6. **P.S. Stephanou**, C. Baig, G. Tsolou, M. Kröger, V.G. Mavrantzas, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *6th International Meeting of the Hellenic Society of Rheology,* Athens, Greece, June 26-28 **(2011).**
7. **P.S. Stephanou**, C. Baig, V.G. Mavrantzas, "Generalized viscoelastic model for polymer melts guided by principles of non-equilibrium thermodynamics: Single- and multi-mode

formulations", *7th GRACM International Congress on Computational Mechanics*, Athens, Greece, June 30-July 2 (**2011).**

8. **P.S. Stephanou**, C. Baig, V.G. Mavrantzas, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *17 th International Workshop on Numerical Methods for Non-Newtonian Flows (IWNMNNF 2012)*, Blois, France, March 25-28 (**2012).**
9. **P.S. Stephanou**, C. Baig, V.G. Mavrantzas, "Quantifying chain reptation in entangled polymer melts: Topological and dynamical mapping of atomistic simulation results onto the tube model", *The XVIth International Congress on Rheology (ICR 2012)*, Lisbon, Portugal, August 5-10 (**2012)**
10. V. G. Mavrantzas, **P. S. Stephanou**, N. Stratikis, T. Koukoulas, G. Tsolou, C. Baig, "Rouse theory for polymer rings and comparison with atomistic molecular-dynamics simulations and experimental", *The XVIth International Congress on Rheology (ICR 2012)*, Lisbon, Portugal, August 5-10 (**2012)**
11. **P.S. Stephanou**, V.G. Mavrantzas, "Quantitative predictions of the linear viscoelastic rheological properties of polyethylene entangled melts via modified versions of the dual constraint and Leygue et al. models", *8th Panhellenic Meeting* "*Fluid Flow Phenomena*" *(POH 2012)*, Volos, Greece, November 16-17 (**2012).**
12. **P.S. Stephanou**, V.G. Mavrantzas, G. C. Georgiou, "A generalized differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics", (poster) *8th Panhellenic Meeting «Fluid Flow Phenomena» (POH 2012)*, Volos, Greece, November 16-17 (**2012).**
13. **P. S. Stephanou** and V. G. Mavrantzas, "Multi-scale modelling of polymer melt viscoelasticity: From atoms, to molecules, to primitive paths, to tube models", *9h Panhellenic Chemical Engineers' Conference*, Athens, Greece, May 23-25 **(2013)** [in Greek].
14. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamic", *Thermodynamics 2013*, Manchester, UK, September 3-6 **(2013)**.
15. **P. S. Stephanou** and V. G. Mavrantzas, "Multi-scale modeling of polymer melt viscoelasticity: From atoms, to molecules, to primitive paths, to tube models", (poster) *Thermodynamics 2013*, Manchester, UK, September 3-6 **(2013)**.
16. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamics", (poster), *9th Annual European Rheology Conference (AERC 2014)*, Karlsruhe, Germany, April 8-11 **(2014)**.
17. **P. S. Stephanou** and V. G. Mavrantzas, "Multi-scale modeling of polymer melt viscoelasticity: From atoms, to molecules, to primitive paths, to tube models", *9th Annual European Rheology Conference (AERC 2014)*, Karlsruhe, Germany, April 8-11 **(2014)**.
18. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts", *7th International Meeting of the Hellenic Rheology Society HSR 2014*, Heraklion, Crete, Greece, 7-10 July **(2014)**.
19. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "Continuum model for the phase behaviour, microstructure, and rheology of unentangled polymer nanocomposite melts", *10th Hellenic Polymer Society Conference*, Patras, Greece, 4-6 December **(2014)**.
20. V. G. Mavrantzas, **P. S. Stephanou**, and G. C. Georgiou, "Using nonequilibrium thermodynamics to model the phase behavior, microstructure and rheology of polymer nanocomposite melt", *A Special Rheology Symposium in honor of Professor Roger I. Tanner on the occasion of his 82 nd birthday*, Vathi, Samos, Greece, 29 June-4 July **(2015)**.
21. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A differential constitutive equation for polymer nanocomposites based on principles of non-equilibrium thermodynamic", *7th International Workshop and Summer School on Nonequilibrium Thermodynamics (IWNET 2015)*, Hilvarenbeek, The Netherlands, July 5-10 **(2015)**.
22. **P. S. Stephanou**, I. Ch. Tsimouri, and 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, Zurich, Switzerland, April 1 **(2016)**.

23. **P. S. Stephanou**, and M. Kröger, "Shear rheology of polymer melts based on a Fokker-Planck equation exhibiting both reptation and orientational diffusion", *20th Anniversary Meeting of the European Society of Rheology*, Zurich, Switzerland, April 1 **(2016)**.
24. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Non-equilibrium thermodynamics modelling and atomistic simulation of polymer nanocomposites", *11th Hellenic Polymer Society International Conference*, Heraklion, Crete, Greece, November 3-5 **(2016)**.
25. **P. S. Stephanou**, T. Schweizer and M. Kröger, "The mechanism behind the appearance of undershoots in start-up shear" (poster), *11th Hellenic Polymer Society International Conference*, Heraklion, Crete, Greece, November 3-5 **(2016)**.
26. I. Ch. Tsimouri**,** C. K. Georgantopoulos, **P. S. Stephanou**, and V. G. Mavrantzas, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics" (poster), *11th Hellenic Polymer Society International Conference*, Heraklion, Crete, Greece, November 3-5 **(2016)**.
27. I. Ch. Tsimouri**,** C. K. Georgantopoulos, **P. S. Stephanou**, and V. G. Mavrantzas, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics", *12th Annual European Rheology Conference (AERC 2017)*, Copenhagen, Denmark, April 3-6 **(2017)**.
28. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *12th Annual European Rheology Conference (AERC 2017)*, Copenhagen, Denmark, April 3-6 **(2017)**.
29. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modelling coupled with NEMD simulations", *Eurofillers Polymer Blends 2017*, Hersonissos, Heraklion Crete, Greece, April 23-27 **(2017)**.
30. C. K. Georgantopoulos, I. Ch. Tsimouri**, P. S. Stephanou**, and V. G. Mavrantzas, "Derivation of modern rheological constitutive models through the use of non-equilibrium thermodynamics" (poster), *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
31. I. Ch. Tsimouri**, P. S. Stephanou**, and V. G. Mavrantzas, "A constitutive rheological model for blood through the use of non-equilibrium thermodynamics", *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
32. **P. S. Stephanou**, D. G. Tsalikis, P. V. Alatas, and V. G. Mavrantzas, "Modelling polymer nanocomposites based on the principles of non-equilibrium thermodynamics modelling and the findings of detailed non-equilibrium atomistic simulations", *11h Panhellenic Chemical Engineers' Conference,* Thessaloniki, Greece, May 25-27 **(2017)** [in Greek].
33. **P. S. Stephanou** and V. G. Mavrantzas, "Polymer melt viscoelasticity: from atomistic molecular dynamics simulations to the tube model" (poster), *11^{h} Panhellenic Chemical Engineers' Conference*, Thessaloniki, Greece, May 25-27 **(2017)**.
34. **P. S. Stephanou**, D. G. Tsalikis, E. N. Skountzos, and 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 Rheology Society HSR 2017*, Limassol, Cyprus, 12-14 July **(2017)**.
35. I. Ch. Tsimouri, C. K. Georgantopoulos, **P. S. Stephanou**, and V. G. Mavrantzas, "Derivation of a recently proposed CCR model through the use of non-equilibrium thermodynamics" (poster), *8th International Meeting of the Hellenic Rheology Society HSR 2017*, Limassol, Cyprus, 12-14 July **(2017)**.
36. **P. S. Stephanou** and V. G. Mavrantzas, "Multi-scale modelling of high-MW polymer melt viscoelasticity starting from the atomistic level" (poster), *8th International Meeting of the Hellenic Rheology Society HSR 2017*, Limassol, Cyprus, 12-14 July **(2017)**.
37. I. Ch. Tsimouri**, P. S. Stephanou**, and V. G. Mavrantzas, "A constitutive rheological model for blood through the use of non-equilibrium thermodynamics", *3rd Workshop of Graduates and Post-Docs in Chemical Engineering Sciences (CES-WGP3), Patras, Greece*, 4 October

(2017).

NON-CONFERENCE PRESENTATIONS

1. **P. S. Stephanou**, "A generalized differential constitutive equation based on principles of non-equilibrium thermodynamics", Department of Mathematics and Statistics, University of Cyprus, Nicosia, Cyprus, October 20 **(2013)** [in Greek].
2. **P. S. Stephanou**, C. Baig, and V. G. Mavrantzas, "Development of scale-bridging methodologies for the reliable prediction of the viscoelastic properties of polymer melts", Polymer Physics group, Department of Materials, ETH-Zürich, Zürich, Switzerland, November 26 **(2014)**.
3. **P. S. Stephanou**, "Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics", Info-day for the *VISCOnanoNET* project held at the Department of Mathematics and Statistics, University of Cyprus, Nicosia, Cyprus, December 19 **(2014)**.
4. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A unified description of the phase behavior and rheology of spherical nanoparticles dispersed within a polymeric matrix using non-equilibrium thermodynamics", Department of Mechanical and Process Engineering, Particle Technology Laboratory, ETH Zürich, Zürich, Switzerland, October 9 **(2015)**.
5. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A unified description of the phase behavior and rheology of spherical nanoparticles dispersed within a polymeric matrix using non-equilibrium thermodynamics", Department of Mechanical and Manufacturing Engineering, University of Cyprus, Nicosia, Cyprus, October 15 **(2015)** [in Greek].
6. **P. S. Stephanou**, V. G. Mavrantzas and G. C. Georgiou, "A unified description of the phase behavior and rheology of spherical nanoparticles dispersed within a polymeric matrix using non-equilibrium thermodynamics", Department of Chemistry, University of Cyprus, Nicosia, Cyprus, March 30 **(2016)** [in Greek].
7. **P. S. Stephanou**, P. Alatas, D. G. Tsalikis, V. G. Mavrantzas and G. C. Georgiou, "Multiscale modelling approach to the rheological behaviour of polymer nanocomposites: Nonequilibrium thermodynamics modeling coupled with NEMD simulations", Department of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology, Lemesos, Cyprus, October 20 **(2016)** [in Greek].
8. **P. S. Stephanou**, and M. Kröger "Appearance of undershoots when using the tumbling-snake model in startup simple shear flow", Department of Mathematics and Statistics, University of Cyprus, Nicosia, Cyprus, November 23 **(2016)** [in Greek].
9. **P. S. Stephanou** "Modeling the flow and deformation of complex systems using non-equilibrium thermodynamics", Department of Physics, National and Kapodistrian University of Athens, Athens, Greece, January 27 **(2017)** [in Greek].

STUDENT CO-ADVISEMENT AS GRADUATE STUDENT

Master Thesis students

1. Nikos Stratikis (academic advisor: Prof. V.G. Mavrantzas, graduated in **2011**)

Diploma Thesis students

1. Eva Lionta (academic advisor: Prof. V.G. Mavrantzas, graduated in **2010**)
2. Vasilis Georgilas (academic advisor: Prof. V.G. Mavrantzas, graduated in **2010**)

STUDENT CO-ADVISEMENT AS POST-DOCTORAL RESEARCHER

Master Thesis students

1. Ioanna Tsimouri (academic advisor: Prof. V.G. Mavrantzas, to graduate in **2018**)

Diploma Thesis students

1. Ioanna Tsimouri (academic advisor: Prof. V.G. Mavrantzas, graduated in **2016**)
2. Christos Georgantopoulos (academic advisor: Prof. V.G. Mavrantzas, to graduate in **2018**).

REVIEWER FOR SCIENTIFIC JOURNALS

Reviewer for manuscripts submitted for consideration for publication in (also included the impact factor of 2016):

1. Physical Review Letters (PRL) (I.F. 8.462).
2. Soft Matter (I.F. 3.889).
3. Langmuir (I.F. 3.833).
4. Journal of Rheology (I.F. 3.136).
5. Journal of Chemical Physics (I.F. 2.965).
6. Powder Technology (I.F. 2.942).
7. Industrial and Engineering Chemistry Research (I.F. 2.843).
8. Journal of Non-Newtonian Fluid Mechanics (I.F. 2.536).
9. Physical Review E (PRE) (I.F. 2.366).
10. Physics of Fluids (I.F. 2.232).
11. Macromolecular Theory and Simulation (I.F. 2.294).
12. Chemical Physics Letters (I.F. 1.860).

ORGANIZATION OF SCIENTIFIC MEETINGS

1. Assistance Personnel, *4th International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (IWNET),* Rhodes, Greece, September 4-7, **2006**.
2. Assistance Personnel, *15th International Workshop of Numerical Methods for Non-Newtonian Flows*, Rhodes, Greece, June 14-17, **2007**.
3. Member, Organizing Committee, 8th *International Meeting of the Hellenic Society of Rheology (HSR2017)*, Limassol, Cyprus, July 12-14, **2017**.

REFERENCES

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