

## PAVLOS S. STEPHANOU



### *Office*

Associate Professor

Thermodynamics and Transport Phenomena  
Laboratory (T<sup>2</sup>PL)

Department of Chemical Engineering,  
Cyprus University of Technology,  
Corner of Athinon and Anexartisias, 57  
3036 Limassol, CYPRUS  
e-mail: [pavlos.stefanou@cut.ac.cy](mailto:pavlos.stefanou@cut.ac.cy).

Tel.: +357-25002394

Mob.: +357-99-444563

Fax.: +357-25002668

Personal Webpage: <https://pstephanou.wixsite.com/mysite>

ORCID: 0000-0003-3182-0581

Scopus Author ID: 26032382500

Web of Science Researcher ID: M-2260-2019

Research Gate: [https://www.researchgate.net/profile/Pavlos\\_Stephanou](https://www.researchgate.net/profile/Pavlos_Stephanou)

LinkedIn: <https://www.linkedin.com/in/pavlos-stephanou-135521118/>

Google Scholar: <https://scholar.google.com/citations?user=uht8jaMAAAAJ&hl=en>

### LANGUAGES

Fluent in English, Greek

### LEISURE ACTIVITIES

Literature and poetry reading

### PERSONAL INFO

Date of birth: January 14, 1982

Family status: Married, two sons (b. 2014, 2017), one daughter (b. 2019)

Citizenship: Cypriot

### ACADEMIC INTERESTS

Physical Chemistry: Equilibrium Thermodynamics, Statistical Thermodynamics, Non-Equilibrium Thermodynamics, Statistical Mechanics

Materials: Physical and Chemical Processes, Statistical Mechanics of Polymers, Polymer Mechanics and Physics, Nanomaterials, Dynamics of Polymeric Liquids, Polymer Rheology, Fluid Mechanics,

Numerical Analysis: Numerical Methods for Engineers, Finite Difference Method, Finite Element Method.

### RESEARCH INTERESTS

Polymers: Modelling at the mesoscopic and macroscopic level, rheological and dynamical behavior, 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, **8<sup>th</sup> Highest GPA ever recorded**)
- *Diploma thesis:* “Atomistic modelling of the polyelectrolyte membrane Nafion®”
- *Advisor:* Prof. Vlasis G. Mavrantzas

## EXPERIENCE

### Associate Professor (August 2024 – Today)

Department of Chemical Engineering, Cyprus University of Technology, Cyprus

### Assistant Professor (September 2019 – July 2024)

Department of Chemical Engineering (until December 2020 named Department of Environmental Science and Technology), Cyprus University of Technology, Cyprus

### Post-Doctoral Researcher (August 2018 – August 2019)

Novamechanics Ltd, Nicosia, Cyprus

#### **Research Outline**

- Derivation of a generalized constitutive model for the transport of drug-carrying nanoparticles in blood based on principles of non-equilibrium thermodynamics
- Solving modifications of the Curtiss-Bird model using Stochastic Dynamics solvers (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. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z).
- Multi-scale modelling of polymer-based nanocomposites (with Prof. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z).

### Post-Doctoral Researcher (Special Scientist) (September 2016 – July 2018)

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 Stochastic Dynamics solvers (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. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z).
- 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 Stochastic Dynamics solvers.
- 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, Switzerland).
- Derivation of a generalized constitutive model for blood based on principles of non-equilibrium thermodynamics (with Prof. V.G. Mavrantzas, LSTM, DCE, UP, Greece and DME, ETH-Z).

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 using Finite Elements modeling” with A. Anastasiou, Project undertaken during “Advanced Numerical Methods” course, Fall **2008**.

## TEACHING

*Undergraduate Courses (as Assistant Professor)*

- “Energy Transport Phenomena” CEN 308, Department of Environmental Science and Technology (DEST) now Department of Chemical Engineering (DCE), CUT, Fall **2019, 2020,2021**.
- “Chemical Processes” CEN 210, DEST, CUT, Fall **2019**.
- “Lab Chemical Processes” CEN 210E, DEST, CUT, Fall **2019**.
- “Mass Transport Phenomena” CEN 207, DCE, CUT, Spring **2020,2021,2022**.
- “Unit Operations I” CEN 209, DCE, CUT, Spring **2020,2021,2022,2023,2024,2025**.
- “Unit Operations Lab I” CEN 209E, DCE, CUT, Spring **2020,2021**.
- “Unit Operations II” CEN 327, DCE, CUT, Fall **2020,2021,2022,2023,2024**
- “Unit Operations Lab II” CEN 327E, DCE, CUT, Fall **2020**
- “Operations Lab II” CEN 403, DCE, CUT, Fall **2021,2022,2023**
- “Processes Design and Control” CEN 406, DCE, CUT, Fall **2022**
- “Transport Phenomena I: Fluid Mechanics” CEN 207, DCE, CUT, Spring **2023,2024,2025**.
- “Transport Phenomena II: Heat and Mass Transfer” CEN 312, DCE, CUT, Fall **2023,2024**

*Additional Teaching Experience (as Assistant Professor)*

- Teaching the courses “Rheological Properties of Petroleum and Lubricants” and “An Introduction to fractional distillation” to army officers (February and April **2022, 2023,2024,2025**)

*Undergraduate Courses (as Special Scientist-Postdoctoral Researcher)*

- “Mathematics II” MEM 102 (Multivariate Calculus), 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, 2018**.
- “Dispersion Models” EST 401 (Atmospheric dispersion models), Department of Environmental Science and Technology (DEST), CUT, Fall **2018**.
- “Mass Transport Phenomena” CEN 207, DEST, CUT, Spring **2019**.
- “Applied Thermodynamics II” CEN 305, DEST, CUT, Spring **2019**.

*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**).

#### Informal Teaching

Taught (in weekly group meetings in **2006**) with Dr. Chunggi Baig (now 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), 23 November **2015**, <https://www.youtube.com/watch?v=SX1OC-xs9zA> (in Greek).
- Marie Skłodowska-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).
- The only postdoctoral researcher to receive a DIDAKTOR fund (equivalent to Marie Skłodowska-Curie funding on a national level) by the Cyprus Research Promotion Foundation twice (in two consecutive calls).<sup>1</sup>
- Alternate Member of the Audit Committee of the Hellenic Society of Rheology (HSR) (July **2022**-to date).
- Member of the editorial board, of the journal Polymers (MDPI), IF 4.967 <https://www.mdpi.com/journal/polymers/editors> (Since Sep. **2022**).
- Advisory Board Member of Preprints (Preprints is a multidisciplinary preprint platform that accepts articles from all fields of science and technology, given that the preprint is scientifically sound and can be considered part of academic literature) (Since Sep. **2023**)
- Tasos C. Papanastasiou Award, Hellenic Society of Rheology (HSR) June 13th, **2025**. [[Announcement 1](#), [Announcement 2](#), [Announcement 3](#)]

#### **PROFESSIONAL AFFILIATIONS**

- Member, Hellenic Society of Rheology (HSR) (2011-today).
- Member, European Society of Rheology (ESR) (2014-today).
- Member, Society of Rheology (SOR) (2019-today).
- Member, American Chemical Society (ACS) (2018-2019).

#### **PARTICIPATION IN RESEARCH AND DEVELOPMENT PROJECTS**

##### **As Post-Doctoral Researcher at Dep. Of Mathematics, UCY And Dep. Materials, ETH Zurich**

##### **VISCONanoNET**

- Marie Curie Reintegration grant titled: *Modelling the viscoelasticity of polymer-based nanocomposites guided by principles of non-equilibrium thermodynamics*

---

<sup>1</sup> Katerina Karakasidou, Research and Innovation Foundation (RIF), personal communication via email, August 3rd 2018

- Funding Body: EC
- 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
- Role: Proposal writing, Conducting Research

*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
- Website: <http://euclid.mas.ucy.ac.cy/~visconan/>
- Role: Proposal writing, Conducting Research

*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: KOYATOYPA/BP-NE/0415/01
- Partners: Univ. Cyprus
- RPF contribution: 35 k€
- Duration: 09/2016 – 05/2018
- Project coordinator: P.S. Stephanou.
- Role: Proposal writing, Conducting Research
- Website: <http://euclid.mas.ucy.ac.cy/~multiscalepnc/index.html>

*ViP-MeDiCinA*

- National grant titled: *An in-silico Virtual-Patient Modelling of the effective transport of Drug-Carrying particles to treat Atherosclerosis*
- Funding Body: Cyprus Research Promotion Foundation
- Contract No: POST-DOC/0916/0197
- Partners: NovaMechanics Ltd (coordinator), Univ. Cyprus, Univ. Patras
- RPF contribution: ~160 k€
- Duration: 08/2018-07/2020 [terminated on 08/2019 due to my employment at CUT]
- Project coordinator: A. Afantitis
- Role: Proposal writing, Conducting Research

**As Assistant Professor at Dep. Chemical Engineering, CUT**

*NET-CST*

- Grant titled: *A non-equilibrium thermodynamics approach to couple stress fluids*
- Funding Body: Cyprus University of Technology (Starting Grant)
- Duration: 01/03/2020-30/04/2022
- Budget: 38.5 kEuro
- Project coordinator: Dr Pavlos S. Stephanou
- Role: Proposal writing, Conducting research guidance

ProMoTox

- National grant titled: *Prognostic Modeling for Cardiovascular Implant Toxicology*
- Funding Body: Cyprus Research and Innovation Foundation (The «Industrial Property» program aims to the increase of the number of patents and industrial designs that are filed by Cypriot entities, with the long-term term objective of maximising the benefits generated by the results of research and innovation activities.)
- Contract No: INDUSTRIAL-PROPERTY/0717/0034
- RPF contribution: 10 k€
- Duration: **06/2021-10/2022**
- Project coordinator: Dr. A. Anayiotos
- Role: Co-inventor of the patent

Super4-quark

- Grant titled: *New directions in the Physics of Elementary Particles: SuperSymmetry and Four-quark Quantum operators*
- Funding Body: Cyprus University of Technology (“METADIDAKTOR” Grant for funding post-doctoral researchers)
- Duration: **01/08/2022-31/07/2023**
- Budget: 19.8 kEuro
- Project coordinator: Dr Marios Kosta
- My role: Academic Coordinator in CUT

SUGARS

- Grant titled: *Optimized in silico sour gas processing for offshore deepwater gas technology applications at the Eastern Mediterranean region.*
- Funding Body: Cyprus Research and Innovation Foundation (PHD IN INDUSTRY Grant for funding research projects implemented by the Ph.D. candidate employed in an enterprise while registered at a PhD Programme)
- Contract No: PHD IN INDUSTRY/1222/0123
- Consortium: Cyprus Hydrocarbons Company (CHC) (coordinator), Cyprus University of Technology
- Duration: **01/10/2023-30/09/2026**
- Budget: 150 kEuro
- Project coordinator: Dr. Nicolas Droushiotis (CHC)
- My role: Proposal writing (with Dr.Droushiotis), Conducting research guidance in WP4 and WP5.

CRaFTC

- Grant titled: *Cyprus Rheology And Fluidics Technology Centre.*
- Funding Body: Cyprus Research and Innovation Foundation (SMALL SCALE INFRASTRUCTURES Grant that concerns the funding of projects aimed at creating new large-scale research infrastructures that will be used for the implementation of a research project by the Consortium)
- Contract No: SMALL SCALE INFRASTRUCTURES/1222/0181
- Consortium: Cyprus University of Technology (coordinator), University of Cyprus, CYENS Centre of Excellence, EMBIO Diagnostics Ltd
- Duration: **30/12/2023-30/06/2026**
- Budget: 700 kEuro
- Project coordinator: Dr. Efstatios Kaliviotis (CUT)
- My role: Proposal writing (minor contribution, with Dr Kaliviotis and others), Conducting research guidance in WP3 (Task 3.3) and WP4 (Task 4.2).

ID: I-2023-10808

- Grant titled: *Casting the Future: Optimizing the extraterrestrial 3D printing of cement-based*

*structures*

- Funding Body: European Space Agency's (ESA) Discovery Programme via the EISI (ESA Initial Support for Innovation) implementation mechanism
- Contract No: EISI AGREEMENT ID: I-2023-10808
- Consortium: Cyprus University of Technology
- Duration: **01/09/2024-01/09/2027**
- Budget: 90 kEuro (covering the salaries of a PhD student)
- Project coordinator: Dr. Pavlos S. Stephanou.
- My role: Proposal writing, Project Management and Dissemination in WP1-WP2, Conducting research guidance in WP3-WP5.

**As Associate Professor at Dep. Chemical Engineering, CUT**

**PROPOSALS GRANTED BUT NOT STARTED**

*AtherOpt*

- Grant titled: *Optimizing the design of Drug-Carrying particles to treat Atherosclerosis via in silico virtual-patient modeling*.
- Funding Body: Cyprus Research and Innovation Foundation (PHD IN INDUSTRY Grant for funding research projects implemented by the Ph.D. candidate employed in an enterprise while registered at a PhD Programme)
- Call No: PHD IN INDUSTRY/1123
- Evaluation Score: 14.52/15.00 (ranked 1<sup>st</sup> out of 31 proposals)
- Consortium: NovaMechanics Ltd (coordinator), Cyprus University of Technology
- Intended Budget: 150 kEuro
- My role: Proposal writing.
- Reason for not starting: The PhD student named in the proposal was Ms Amalia Ioannou whose PhD had already started being funded by ESA (ID: I-2023-10808). As such, given that it was not allowed to substitute for the PhD student who would participate and be funded, the proposal never materialized.

**PATENTS**

- 1) Konstantinos Kapnisis, Pavlos S. Stephanou, and Andreas Anayiotos, [\*Physiologically based toxicokinetic \(PBTK\) modeling for implant toxicology\*](#), WO2022248703A2, WIPO (PCT).

**PARTICIPATION IN COST ACTIONS**

*EUTOPIA*

- COST Action grant titled: *European Topology Interdisciplinary Action (EUTOPIA)*
- Funding Body: EC
- Contract No: CA17139
- Duration: **18/10/2018-17/10/2022**
- Project coordinator: Dr Luca Tubiana (Univ. Trento, Italy)

*MecaNano*

- COST Action grant titled: *European Network for the Mechanics of Matter at the Nano-Scale (MecaNano)*
- Funding Body: EC
- Contract No: CA21121
- Duration: **30/09/2022-29/09/2026**
- Project coordinator: Prof Benoit Merle (Univ. Kassel, Germany)

**PARTICIPATION IN COMPUTATIONAL PROJECTS (to receive computational resources)**

- 1) *Validation of the Zimm model for ring systems in theta solvents using Molecular Dynamics simulations, 01/04/2023-31/03/2024*, The Cyprus Institute National HPC System Cyclone, Total number of CPU core-hours received: 472320.

## CERTIFICATES

- 1) Continuing Professional Development Program for Academic Staff, "Design and Development of Hybrid, Blended, and Distance Learning Programs". Organized by the Learning Enhancement and Development Network of the Cyprus University of Technology during the academic year 2024-2025. Total workload: 20 hours

## RESEARCH ACTIVITIES

A major theme of my research work has been the development of reliable constitutive models for describing the dynamics and equilibrium (i.e., no imposed flow) and flow behavior of complex polymeric fluids. At equilibrium, I derive and solve theories of polymer dynamics using simple molecular models of different polymeric systems (e.g., ring polymers). The aim is to understand the properties of various polymeric systems and to provide the avenue to design tailor-made systems with improved properties. In this case, we consider simple models that can be solved analytically or numerically, however, as we mention below, we strive to always compare the predictions of these theories with (equilibrium) Molecular Dynamics (MD) simulations. On the other end, under the imposition of a flow field, 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 have expanded the complex fluids to which I employ NET to derive constitutive models, such as thixotropic fluids, blood, shear thickening fluids, micellar systems, petroleum oil-in-water emulsions, cement pastes,**

In most cases, the resulting constitutive equations contain parameters whose values are not known. To overcome this, I resort to atomistic simulations, both (equilibrium) 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 execute atomistic MD and NEMD simulations to simulate the actual chemical and biological system under exact processing conditions to 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 periods 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.

More recently, I have also been involved in developing modeling approaches for biological systems, such as predicting the deposition of a substance in various organs in our body and describing the process used by specific organisms to produce important products, i.e., bioreactors.

Below, I provide a more elaborate listing of the major problems that I have researched. Citations refer to the reference list provided in the section “Publications in Refereed Journals” that follows.

### MAJOR PROBLEMS ADDRESSED

#### A) POLYMERIC SYSTEMS

##### 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<sup>2</sup> or obtained through Non-Equilibrium Molecular Dynamics (NEMD) simulations in shear and planar elongation (see Fig. A1).

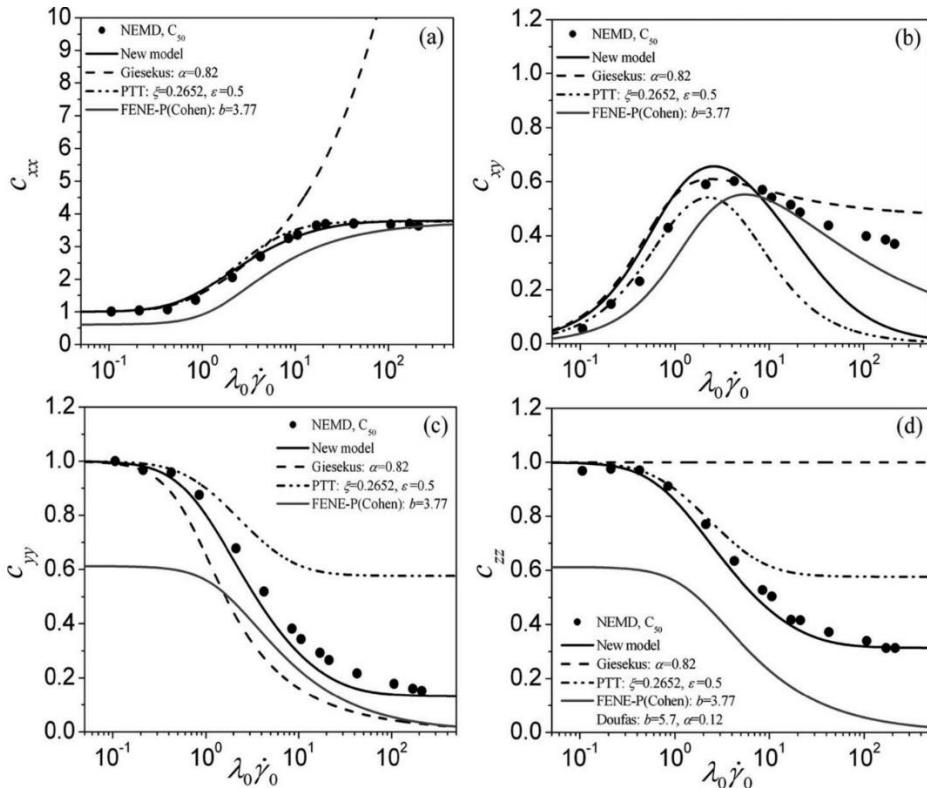


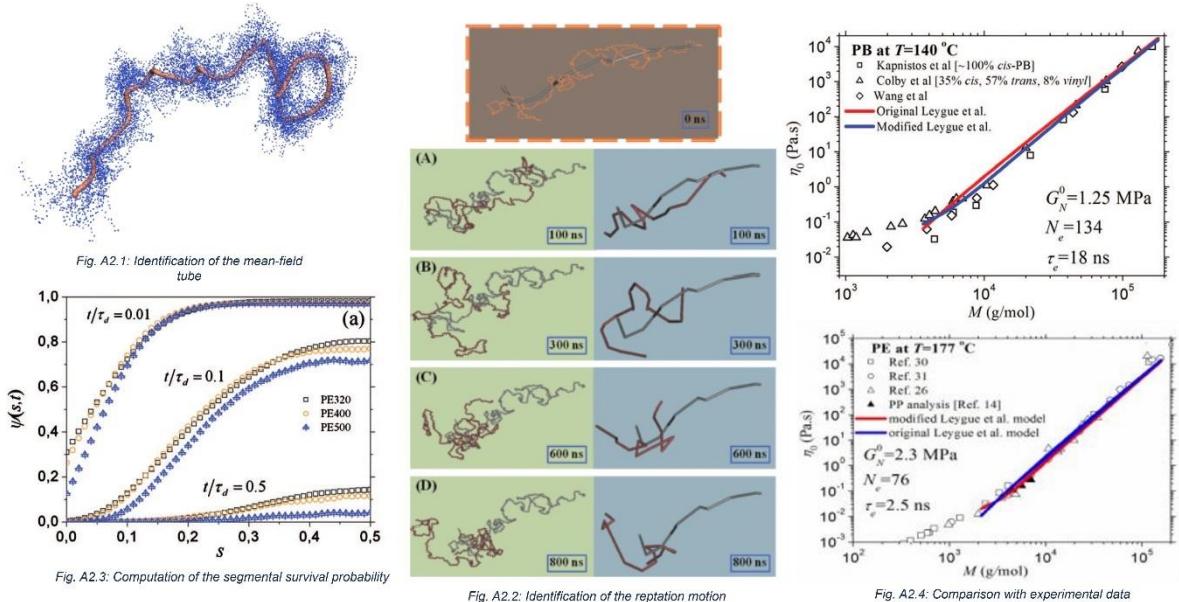
Fig. A1: Model predictions for the nonzero components of the conformation tensor in steady shear for the  $C_{50}H_{102}$  polyethylene melt along with comparison with the NEMD simulation results and the predictions of other models based on best fits

##### 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

<sup>2</sup> P. S. Stephanou, C. Baig, V.G. Mavrantzas, and J. Den Doelder, (2011) (report)

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 (Fig. A2.1) and then documenting chain motion in terms of a curvilinear diffusion inside the effective tube around the coarse-grained chain contour (Fig. A2.2). 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  $t$  (Fig. A2.3). 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 [usually expressed in the form of a partial differential equation, similar to the diffusion equation, of  $\psi(s,t)$ ]. 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 (Fig. A2.4).



### 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 in 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  $C_{24}$  up to  $C_{400}$  at temperature  $T=450$  K and  $P=1$  atm, especially for rings with chain length between  $C_{50}$  and  $C_{170}$ ). 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,  $\tau_p$ , the monomeric friction coefficient,  $\zeta$ , and the zero-shear rate viscosity,  $\eta_0$ , on chain length  $N$ ) is that PE ring melts follow approximately Rouse-like dynamics even when their chain length is as long as  $C_{400}$ ; this is more than twice the characteristic crossover chain length ( $\sim C_{156}$ ) 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) *Constitutive equations for Entangled polymer melts and solutions guided by principles of non-equilibrium thermodynamics* [Refs.: 14,24]

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  $\alpha$ , 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  $\beta_{\text{CCR}}$  to values strictly greater than one ( $\beta_{\text{CCR}} > 1$ ) and the new parameter  $\alpha$  to values in the interval  $0 \leq \alpha \leq 1 - \beta_{\text{CCR}}^{-1}$ . 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. Our most recent efforts are focused on extending this model so as it allows for a decreasing entanglement density (manuscript soon to be submitted).

#### 6) *Predicting undershoots in the transient viscosity of entangled polymer melts and concentrated polymer solutions* [Refs.: 13,15-16, 18-19,23]

It has been about a decade ago that undershoots in the transient viscosity of polymer solutions, when startup shear flow is applied, were observed for the first time and more recent rheological measurements further illustrate that such a dumping behavior is absent in the transient normal stress coefficients (Ref. 15). Furthermore, the steady-state extensional viscosity of dense polymeric liquids in fast elongational flows is known to be peculiar in the sense that for entangled polymer melts it monotonically decreases – whereas for concentrated polymer solutions it increases – with increasing strain rate beyond the inverse Rouse time.

We have demonstrated that the Curtiss-Bird model (that we coin the tumbling-snake model), a bead-link chain kinetic theory for entangled polymer melts and concentrated solution, has the necessary capacity to qualitatively predict the appearance of undershoots in the transient viscosity at large shear rates under startup shear and its absence in the normal stress coefficients of concentrated polymeric solutions (Fig. A6.1), when supplemented by a non-constant link-tension coefficient that we relate to the nematic order parameter (Refs. 15-16). To solve the model, we translated the evolution equation for the probability distribution function, the so-called “single-link” distribution function, to an ordinary stochastic differential equation (SDE). The observed phenomena are attributed to the tumbling behavior of the links, triggered by rotational fluctuations, on top of reptation. Naturally, such a dumping behavior

should be absent in elongation flows, without any further adjustments (Ref. 18). In addition, by having the friction tensor increasingly become isotropic at large strain rates as the polymer concentration decreases, the model (Ref. 18) is seen to capture the experimentally observed behavior noted in the steady-state extensional viscosity (Fig. A6.2). Overall, our work demonstrates the capacity of the tumbling-snake model to improve our microscopic understanding of the rheology of entangled polymer melts and concentrated polymer solutions (Refs. 14-16,18). More recently, we have derived, using non-equilibrium thermodynamics, a constitutive model that also shows the potential to predict accurately the appearance of a dumping behavior (Ref. 24)

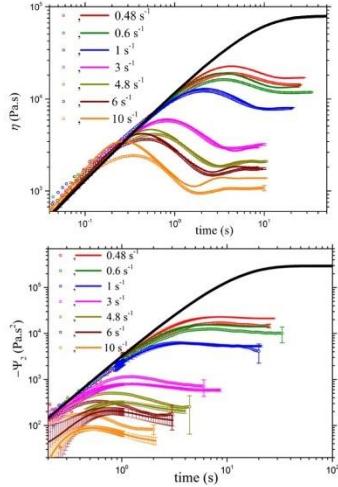


Fig. A6.1: Accurate prediction of the appearance of undershoots in shear viscosity and its absence in normal stresses.

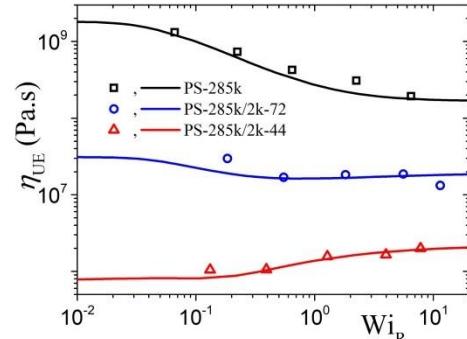
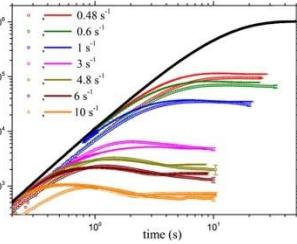


Fig. A6.2: We manage to accurately predict the increase of the steady-state extensional viscosity for concentrated polymer solutions it increases with increasing strain rate beyond the inverse Rouse time

## B) POLYMER NANOCOMPOSITES

### 1) 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 worldwide 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  $\mathbf{C}$ , 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  $\mathbf{a}$  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 (Fig. B1.1 left), and to reliably fit measured rheological data for their shear and complex viscosity over large ranges of volume fractions and deformation rates (Fig. B1.2 right). 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. (Fig. B1.1 right). Overall, our model predicts that flow enhances miscibility, since the corresponding miscibility window opens up for non-zero shear rate values (Fig. B2.1 left).. 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, [https://www.youtube.com/watch?v=SX1OC\\_xs9zA](https://www.youtube.com/watch?v=SX1OC_xs9zA), in Greek) in the context of which Dr. Stephanou has received a research grant (equal to 35 kEuros) from the Research Promotion Foundation (RPF) of Cyprus.

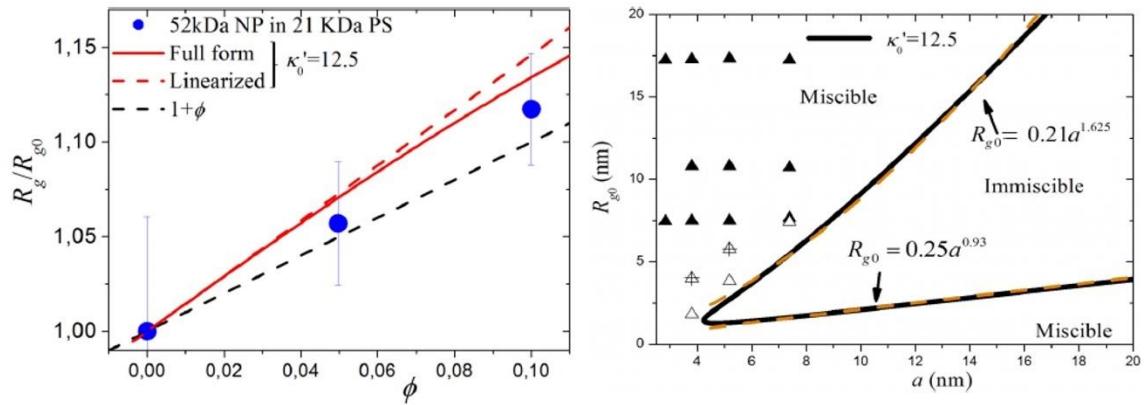


Fig. B1.1: Predictions at equilibrium: variation of the polymer radius-of-gyration with NP volume fraction and comparison with experimental data (left) and the phase behavior of polymer nanocomposites and comparison with experimental data (right)

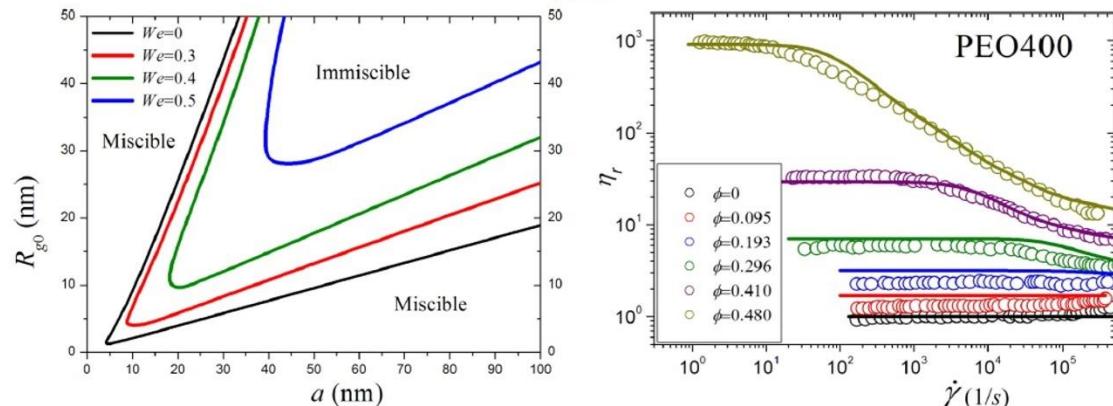


Fig. B1.2: Predictions under flow for the phase behaviour under simple shear flow (left) and the relative viscosity of a PNC as a function of the imposed shear rate (for several volume fractions of nanoparticles) and comparison with the experimental data (right)

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. More recently, we have demonstrated how to provide a more general framework for the modeling of soft-soft nanocomposites, novel nanocomposites systems that exhibit both a viscoelastic and an elastic behavior (Ref. 31).

**2) Multi-scale modeling of polymer nanocomposites [Refs.: 21]**

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).

**3) Deriving and benchmarking the Rouse model suitably adapted for polymer chains adsorbed by one or both of their ends onto the surface of nanoparticles [Refs.: 28]**

We have derived and solved the Rouse model by adapting it to consider polymer chains that are adsorbed by one or both of their ends onto the surface of nanoparticles. We have also showcased the validity of the model by using molecular dynamics simulations to offer a quantitative description of the local structure and microscopic dynamics in attractive polymer nanocomposite melts using a poly(ethylene glycol) (PEG)/silica nanocomposite as a model system. The simulations reveal significant differences in the structural and dynamic properties of the PEG/silica nanocomposite melts studied for different terminal groups (hydroxyl versus methoxy) of the PEG chains, originating from the different ways that polymer chains adsorb on the silica surface: hydroxyl-terminated PEG chains are adsorbed by their ends giving rise to a brush-like structure, whereas methoxy-terminated ones are adsorbed equally probably along their entire contour, thus resulting in better packing of adsorbed segments. Due to the dense interfacial layer that develops in both cases, the diffusive behavior of free chains is also affected (it slows down compared to that in the corresponding pure PEG melt), especially in the nanocomposite where PEG chains are terminated with hydroxyl groups. Direct comparison of simulation and theoretical predictions (without any free parameter as all parameters needed were obtained directly from the atomistic simulations) with previously reported experimental data in the literature for the dynamic structure factor [Glomann et al., *Phys. Rev. Lett.* 2013, 110, 178001] for the same systems under the same temperature and pressure conditions reveals excellent agreement.

**C) PETROLEUM INDUSTRY-RELATED TOPICS**

**1) The rheology of drilling fluids from a non-equilibrium thermodynamics perspective [Ref.: 20]**

Drilling fluids are usually suspensions of plate-like (clay) particles, such as bentonite which is largely composed of the mineral montmorillonite. Their use in drilling operations is multifunctional, including removing rock from the hole, cooling and cleaning the bit, etc. For drilling fluids to bear the capacity to perform these crucial functions, their rheological properties should be finely tuned, since the failure to do so results in enormous financial losses. The rheological behavior of drillings fluids is usually described by simplistic constitutive equations, such as the Casson or the Herschel- Bulkley models, and the power-law model. Despite the overwhelming data highlighting the significance of their use in numerous fields, they fail to produce normal stresses, whose importance in drilling operations has only recently attracted attention.

In this work, we introduce a continuum model for predicting the rheological behavior of drilling fluids with plate-like suspensions (Fig. C1.1), based on the Hamiltonian formulation of transport phenomena for fluids with a complex microstructure. which, by construction, guarantees consistency with the laws of thermodynamics. It allows for the accurate prediction of normal stresses in addition to shear viscosity (Fig. C1.2). This is the take-home milestone of the present contribution: the model presented allows for non-vanishing predictions for both normal stresses, a feature that makes it unrivaled to all other constitutive models routinely employed in the field. If we aspire to optimize drilling operations, the successful prediction of normal stresses for drilling fluids is paramount. It is therefore expected that its use in CFD calculations, instead of the aforesaid simplified models, will certainly allow for a more reliable and accurate (i.e. closer to actual borehole conditions) optimization of drilling operations. Our current efforts are focused on extending this model to tackle drillings fluids that present a thixotropic behavior, by far the majority of drilling fluids

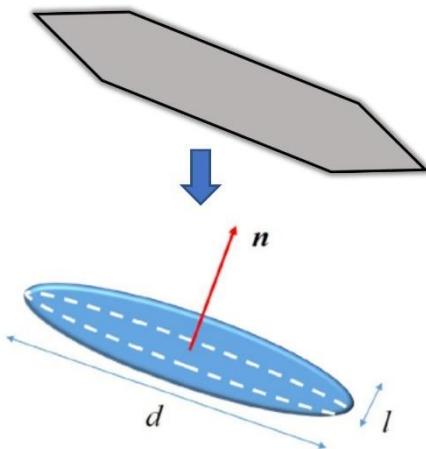


Fig. C1.1: We treat a montmorillonite platelet (up) as an oblate particle with thickness  $l$  and diameter  $d$  (below)

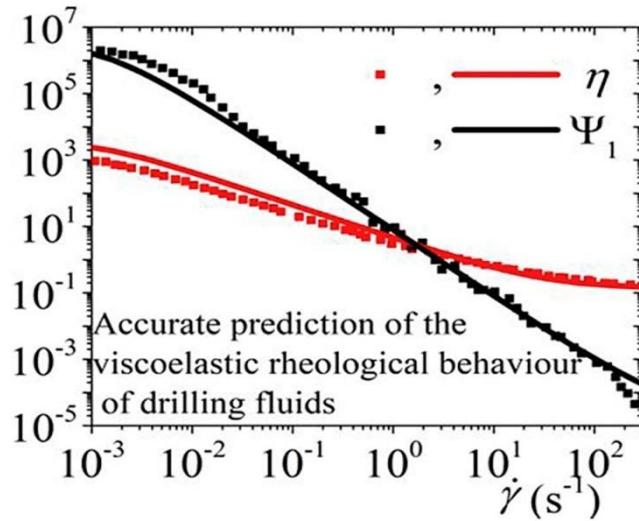


Fig. C1.2: We manage to accurately predict the viscoelastic rheological behavior of drilling fluids

## D) BLOOD AND NANOPARTICLES IN BLOOD

### 1) Constitutive rheological models for non-agglomerating and agglomerating blood derived from nonequilibrium thermodynamics [Refs.: 17, 22, 26-27]

Many cardiovascular diseases leading to severe pathological conditions or even death are often associated with unusual hemodynamic behavior in the circulatory system. For example, intense red blood cell (RBC) aggregation (RBCs tend to aggregate in the presence of plasma proteins, forming structures known as rouleaux) and hyperviscosity syndrome are observed in many pathological conditions altering the transport properties of blood. Owens and coworkers considered blood as an ensemble of rouleaux, each rouleau modeled as an elastic dumbbell (Fig. D1.1). This model drew ideas from the temporary polymer network theory to account for rouleau aggregation and disaggregation. However, it has not been checked for thermodynamic consistency.

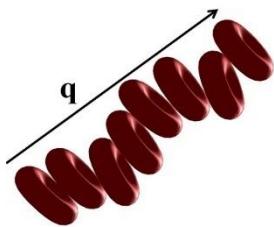


Fig. D1.1: Schematic representation of a rouleau and its corresponding end-to-end vector

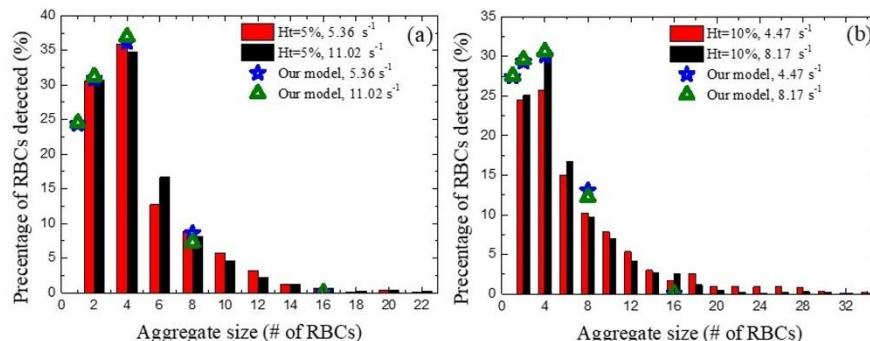


Fig. D1.2: We manage to predict the experimental data for the rouleau size distribution for blood samples under the following conditions: (a)  $Ht = 5\%$  and shear rate  $5.36$  and  $11.02$   $s^{-1}$ , and (b)  $Ht = 10\%$  and shear rate  $= 4.47$  and  $8.17$   $s^{-1}$ .

We derived a constitutive rheological model for human blood which accounts for the formation and dissociation of rouleaux using the generalized bracket formulation of non-equilibrium thermodynamics by following the variables employed by Owens and coworkers. The thermodynamic nature of our model allows for the reaction rates to depend on the instantaneous conformation of the rouleaux. The final set of evolution equations for the microstructure of each rouleau and the expression for the stress tensor turn out to be very similar to those of Owens and co-workers. However, by explicitly considering a mechanism for the formation and breakage of rouleaux, our model further provides

expressions for the aggregation and disaggregation rates appearing in the final transport equations, which in the kinetic theory-based network model of Owens were absent and had to be specified separately. The predictions of our model compare reasonably well with available experimental data on the size distribution of rouleaux (Fig. D1.2).

More recently, we proposed a new model that accounts for the deformability of non-agglomerating RBCs by modeling them as deformed droplets with a constant volume (Ref. 26). Since RBCs are merely droplets with the inner fluid exhibiting a higher viscosity than that of the outer one, RBCs are described by a conformation tensor constrained to have a constant determinant (volume). The model predicts the second normal stress coefficient in steady-state simple shear flow to first shear thicken and then shear thin, which is an unexpected behavior. We show that the new model can address the deformability of isolated (very low hematocrit) RBCs in simple shear and the shear viscosity of non-aggregating blood. Then, we extended this model (Ref. 27) to agglomerating RBCs by properly characterizing the network formed by RBCs under small shear rates, in an average sense. Relative to our previous model, which addresses the rheological behavior of non-aggregating deformable RBCs, one additional structural variable,  $\lambda$ , to properly characterize the network formed by RBCs. The new model predicts a yield shear stress, in accord with experimental data, but also predicts non-vanishing yield normal stresses.

## 2) A Constitutive rheological model predicting the rheological response of rigid particles in blood derived from nonequilibrium thermodynamics [Ref.: 30]

In the past few decades, nanotechnology has been employed to provide breakthroughs in the diagnosis and treatment of several diseases using drug-carrying particles. In such an endeavor, the optimal design of drug-carrying particles is paramount, which necessitates the use of an accurate and trustworthy constitutive model in computational fluid dynamics simulators. We recently introduced a continuum model for elaborating on the rheological implications of adding particles in blood. RBCs are modeled as deformed droplets (following our work in Refs. 26 and 27) with a constant volume that are able to aggregate, whereas particles are considered rigid spheroids (following our work on polymer nanocomposites) 0. The model predictions are compared favorably against rheological data for both spherical and non-spherical particles immersed in non-aggregating blood.

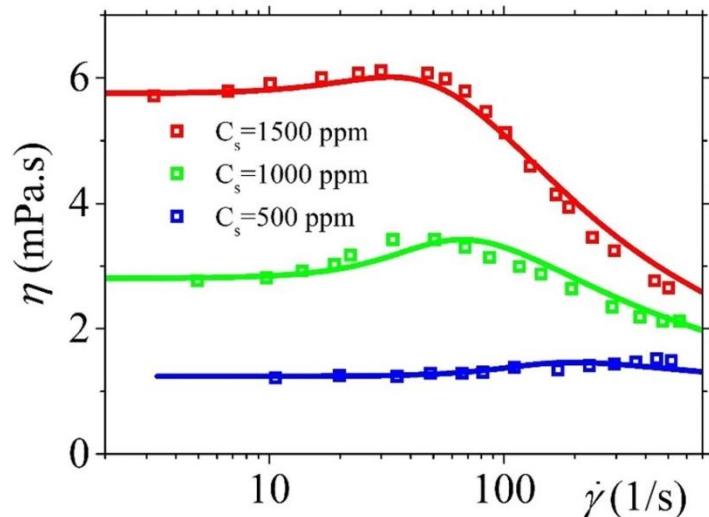


Fig. E1: Comparison of the model predictions for the shear viscosity with the experimental rheological data of three ODMAO, shear-thickening, solutions

## E) SHEAR-THICKENING FLUIDS

### 1) A Constitutive rheological model predicting the rheological response of shear-thickening fluids derived from nonequilibrium thermodynamics [Ref.: 29]

During the past few decades, the interest in understanding the peculiar rheological behavior of shear-thickening fluids has increased due to their potential use in various commercial applications, such as bulletproof vests. We have derived a continuum model to predict the rheological behavior of shear-thickening polymer solutions using non-equilibrium thermodynamics by using a scalar structural varia-

ble that characterizes the formation of the shear-induced structure at sufficiently high shear rates, and a conformation tensor that characterizes the deformation of the polymer segments. The model predicts the exhibition of a shear-thickening behavior for all steady shear flow material functions (shear viscosity and normal stress coefficients), which is then followed by a shear-thinning behavior if finite extensibility or anisotropic effects are considered. We further document that these model predictions are in line with available shear viscosity rheological data for shear-thickening polymer solutions (Fig. E1).

## F) MICELLAR SYSTEMS

### 1) A Constitutive rheological model predicting the rheological response of telechelic micelles derived from nonequilibrium thermodynamics [Ref.: 25]

Associative polymers are solvophilic macromolecules (i.e., they have an affinity for a particular solvent) modified to contain a small number of associating groups, thus characterized by a strong tendency to associate in specific solvents. This feature renders them ideal structures to act as rheology modifiers in products across several fields (health and personal care, enhanced oil recovery, paints and paper coatings, etc.). We have shown how two-species models, already proposed for the rheology of networks of associative polymer solutions, can be derived from nonequilibrium thermodynamics using the generalized bracket formalism. The two species refer to bridges and (temporary) dangling chains, both of which are represented as dumbbells. Creation and destruction of bridges in our model are accommodated self-consistently by assuming a two-way reaction characterized by a forward and a reverse rate constant. Although the final set of evolution equations for the microstructure of the two species and the expression for the stress tensor are similar to those of earlier models based on network kinetic theory, nonequilibrium thermodynamics sets specific constraints on the form of the attachment/detachment rates appearing in these equations, which, in some cases, deviate significantly from previously reported ones. We have also carried out a detailed analysis demonstrating the capability of the new model to describe various sets of rheological data for solutions of associative polymers.

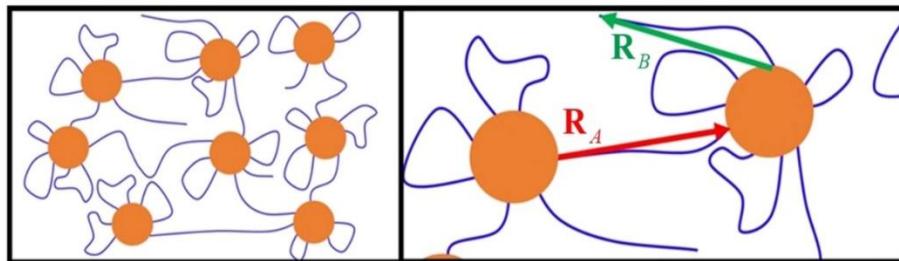


Fig. F1.1: Schematic representation of the process of self-assembly of telechelic polymers into a reversible network.

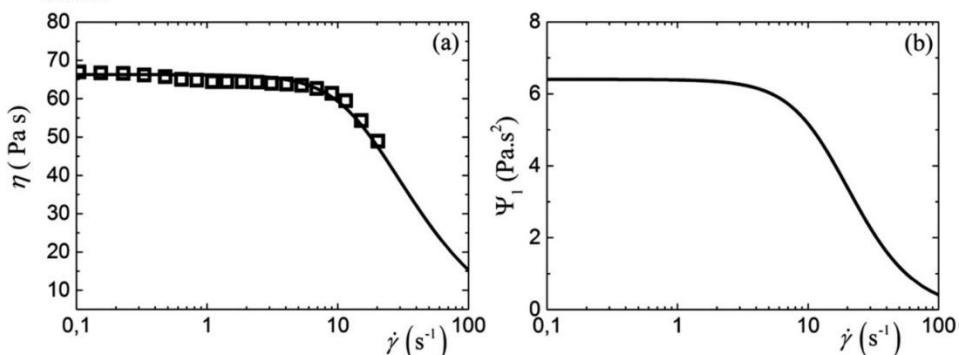


Fig. F1.2: Comparison of the model predictions (lines) for the shear rate dependence of viscosity with measured rheological data. In (b) prediction of the first normal stress coefficient for the same system.

## CURRENT RESEARCH-BRIEF OUTLINE

### 1) Modeling the rheological response of concrete paste [Ref.: 35]

Undoubtedly, cement is one of the most important materials in the construction industry. For its effective use, it is particularly important to fully comprehend the reversible and irreversible rheological behavior of cement paste. When cement is mixed with water, a suspension is initially formed, while as the hydration reactions progress, the cement paste gradually solidifies, making a new irreversible structure.

At the same time, the viscosity of the paste initially decreases with time, while at long times it increases due to the formation of the irreversible structure. We herein introduce a continuum model for predicting the rheological behavior of cement pastes. The model is developed using non-equilibrium thermodynamics, and in particular, the Generalized Brackets formalism, to guarantee model admissibility with thermodynamic laws. To this end, we consider two scalar structural variables: a reversible one,  $\lambda_{rev}$ , characterizing the reversible structure, and an irreversible one,  $\lambda_{irr}$ , characterizing the irreversible structure resulting from the hydrolysis reactions. Also, we consider a tensorial structural variable the conformation tensor  $\mathbf{C}$ , to characterize the deformation of the complex structure. The predictions of the new model compare quite well with available experimental data. It is expected that the use of this model in concrete paste rheology simulators will allow for the in-silico tailor-designing of specific concrete pastes to meet specific needs.

**2) Modeling the rheological response of petroleum oil-in-water emulsions [Ref.: 32]**

During drilling, crude oil is often mixed with water, leading to the formation of water-in-oil (W/O) emulsions. Since these emulsions pose severe flow resistance, such as higher pressure drops, due to their complex fluid rheology, it is important to have in our arsenal a rheological constitutive model that accurately predicts their rheological response. In this work, we propose such a model for W/O emulsions wherein the emulsions are modeled as deformable volume-preserving droplets via the use of a determinant-preserving contravariant second-rank tensor. We use the generalized bracket formalism of non-equilibrium thermodynamics, in order to make sure that the derived model is by construction thermodynamically admissible. An additional scalar structural variable is considered to allow for the prediction of a yield point, following previous work. The predictions of the new model are shown to be in very good agreement with available experimental measurements.

**3) Elucidating the prediction of an asymmetric stress tensor and couple stresses from a NET perspective (theory and molecular simulations) (collaboration with Prof. V. Mavrantzas, DCE, UP, Greece and DME, ETH-Z, Switzerland)**

It has been almost exclusively assumed that the stress tensor employed in Fluid mechanics is symmetric, which implies that there is no interchange between macroscopic and molecular angular momenta. Such a consideration assumes that matter is continuously distributed throughout the body. Although this stands as a reasonable basis for analyzing the behavior of materials at the macroscale level, it fails to do so in cases whence the microstructure size-dependency cannot be neglected, such as polymeric systems or suspensions. In fact, the micro-rotation of freely suspended particles in fluid suspensions gives rise to antisymmetric stress, known as couple stress. In this work, we aim to verify whether the above-mentioned modification of classical fluid mechanics is thermodynamically admissible by using non-equilibrium thermodynamics. The model will also be verified by performing non-equilibrium molecular dynamics (NEMD) simulations using atomistic detail.

**4) Development of a Gene regulatory model to enhance the prediction of bioethanol production by *Saccharomyces Cerevisiae* (collaboration with Prof. M. Koutinas, DCE, CUT)**

The production of biofuels, such as bioethanol from lignocellulosic biomass, constitutes a promising process holding numerous advantages, such as the reduction of fossil fuels and environmental pollution. Alcoholic fermentation is commonly performed by the industrial workhorse *Saccharomyces cerevisiae* which utilizes glucose as the primary energy source. In this work, we predict the kinetics of the microorganism concerning glucose uptake and consumption, by developing a logic model with the use of logic gates. The model will then be parametrized by fitting its predictions against experimental data.

**5) Development of a physiologically based pharmacokinetic model to address the diffusion of toxic substances in humans (collaboration with Prof. A. Anayiotos and Dr K. Kapnisis, DMEMSE, CUT)**

Local and systemic contamination caused by metal ions leaching from medical device materials is a significant and continuing health problem. The increasing need for verification and validation, and the imposition of stringent government regulations to ensure that the products comply with the quality, safety, and performance standards, have led regulatory bodies worldwide, such as the U.S. Food and Drug Administration (FDA), to strongly recommend the use of modeling and simulation tools to support medical device submissions. We have first expanded a previously published PBTK model (and have

provided an analytical solution to it) that predicts Nickel leaching from cardiovascular stents, by considering an additional separate tissue compartment to better resemble normal physiology and by the introduction of time-dependent functions to describe all biokinetic parameters. The new model is exercised in conjunction with state-of-the-art probabilistic, Monte Carlo computational methodology to calculate the predictions' confidence intervals and incorporate variability associated with toxicological biodistribution studies, which was proposed for the first time in the literature. The quantitative consistency of the model-derived predictions is validated against reported data following the implantation of nickel-containing cardiovascular devices in humans and minipigs. This is particularly important as the acquisition of many in vivo samples is prohibitively costly and time-consuming; thus, the confidence intervals should be estimated as accurately as possible to avoid adverse local and systemic health problems. We have further proposed a new methodology for compartmental toxicological risk assessment that can be used for forward or reverse dosimetry. In a more recent publication, the PBTK model has been extended to include the most important tissues/organs and excreta. It also reports on the necessary in vivo data to parameterize it; to the best of our knowledge, this is the very first study that provides in vivo data for so many tissues/organs. Furthermore, a computer-implemented machine learning method is presented to perform a toxicological risk assessment of cardiovascular stents early in their device design cycle.

## PUBLICATION HONOURS

- My article [\*Phys. Fluids\* 32, 103103 \(2020\)](#) was selected by the Editors of *Physics of Fluids* as a featured article (09/2020).
- My article [\*Dynamics\*, 2, 380–398 \(2022\)](#) was selected by the Editor of *Dynamics* to be highlighted on the front page (01/2023).
- My article [\*J. Rheol.\* 67, 849 \(2023\)](#) was selected by the Editor of the *Journal of Rheology* as a Featured article and to be highlighted in [\*Scilight\* 2023, 221109 \(2023\)](#); *Scilights* showcase the most interesting research published in AIP Publishing Journals as selected by the AIP Publishing's journal editors, and written by professional science writers.
- My article [\*Phys. Fluids\*, 35, 113332 \(2023\)](#) was selected by the Editors of *Physics of Fluids* as an "Editor's Pick" article (11/2023).

## PUBLICATIONS IN REFEREEED JOURNALS (\* denotes the corresponding author, link provided)

1. **P. S. Stephanou**, C. Baig, and V.G. Mavrantzas\*, "A generalized differential constitutive equation based on principles of non-equilibrium thermodynamics", [\*J. Rheol.\* 53, 309-337 \(2009\)](#). [Citations: 45]
2. **P. S. Stephanou**, C. Baig, G. Tsolou, 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: 108]
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: 30]
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: 110]
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: 40]
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: 22]
7. **P. S. Stephanou**, C. Baig\*, and 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: 23]

- 8. J. Qin\*, S. T. Milner, **P. S. Stephanou**, and V.G. Mavrantzas, “Effects of Tube Persistence Length on Dynamics of Mildly Entangled Polymers”, *J. Rheol.* **56**, 707-723 (2012). [Citations: 19] selected for the May 15, 2012 issue of Virtual Journal of Biological Physics Research ([www.vjbio.org](http://www.vjbio.org)).
- 9. **P. S. Stephanou**\*, and 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: 17]
- 10. **P. S. Stephanou**\*, and 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: 19]
- 11. **P. S. Stephanou**\*, V.G. Mavrantzas, and G. C. Georgiou, “Continuum Model for the Phase Behavior, Microstructure, and Rheology of Unentangled Polymer Nanocomposite Melts”, *Macromolecules* **47**, 4493–4513 (2014). [Citations: 28]
- 12. **P. S. Stephanou**\*, “How the flow affects the phase behaviour and microstructure of polymer nanocomposites”, *J. Chem. Phys.* **142**, 064901 (2015). [Citations: 21]
- 13. **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: 12]
- 14. **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: 25]
- 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: 28]
- 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**, 174903 (2017). [Citations: 14]
- 17. **P. S. Stephanou**\*, D. G. Tsalikis, E. N. Skountzos, and V. G. Mavrantzas, “Understanding the rheological behavior of polymer nanocomposites: Non-equilibrium thermodynamics modeling coupled with detailed atomistic non-equilibrium molecular dynamics simulations”, *Materials Today: Proceedings* **5**, 27589–27598 (2018) [invited, free-of charge] [Citations: 2].
- 18. I. Ch. Tsimouri, **P. S. Stephanou**\*, and V. G. Mavrantzas, “A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics”, *Phys. Fluids* **30**, 030710 (2018). [Citations: 30]
- 19. **P. S. Stephanou**\*, and M. Kröger\*, “Tumbling-Snake Model for Polymeric Liquids Subjected to Biaxial Elongational Flows with a Focus on Planar Elongation”, *Polymers*, **10**, 329 (2018). [Citations: 6]
- 20. **P. S. Stephanou**\*, and M. Kröger, “From intermediate anisotropic to isotropic friction at large strain rates to account for viscosity thickening in polymer solutions”, *J. Chem. Phys.* **148**, 184903 (2018). [Citations: 7]
- 21. **P. S. Stephanou**\*, “The rheology of drilling fluids from a non-equilibrium thermodynamics perspective”, *J. Pet. Sci. Eng.* **165**, 1010-1020 (2018). (Audioslides presentation: [https://www.youtube.com/watch?v=\\_2U1LQepz50](https://www.youtube.com/watch?v=_2U1LQepz50)) [Citations: 18]
- 22. **P. S. Stephanou**\*, and G. C. Georgiou, “A nonequilibrium thermodynamics perspective of thixotropy”, *J. Chem. Phys.* **149**, 244902 (2018). [Citations: 17].
- 23. **P. S. Stephanou**\*, and M. Kröger\*, “Assessment of the tumbling-snake model against linear and nonlinear rheological data of bidisperse polymer blends”, *Polymers*, **11**, 376 (2019). [Citations: 6].
- 24. **P. S. Stephanou**\*, I. Ch. Tsimouri, and V. G. Mavrantzas, “Simple, Accurate and User-Friendly Differential Constitutive Model for the Rheology of Entangled Polymer Melts and Solutions from Non-Equilibrium Thermodynamics”, *Materials* **13**, 2867 (2020) [invited, free-of charge, Citations: 12].
- 25. **P. S. Stephanou**\*, I. Ch. Tsimouri, and V. G. Mavrantzas, “Two-species models for the

rheology of associative polymer solutions: Derivation from nonequilibrium thermodynamics”, *J. Rheol.* **64**, 1003 (2020). [Citations: 11].

26. **P. S. Stephanou\***, and I. Ch. Tsimouri, “A constitutive hemorheological model addressing the deformability of red blood cells in Ringer solutions”, *Soft Matter* **16**, 7585 (2020). [Citations: 7].

27. **P. S. Stephanou\***, “A constitutive hemorheological model addressing both the deformability and aggregation of red blood cells”, *Phys. Fluids* **32**, 103103 (2020). [Selected as Featured article, Citations: 13] [Erratum: *Phys. Fluids* **33**, 039901 (2021)].

28. E. N. Skountzos,\* D. G. Tsakiris, **P. S. Stephanou**, and V. G. Mavrantzas, “Individual Contributions of Adsorbed and Free Chains to Microscopic Dynamics of Unentangled poly(ethylene Glycol)/Silica Nanocomposite Melts and the Important Role of End Groups: Theory and Simulation”, *Macromolecules* **54**, 4470–4487 (2021). [Citations: 15].

29. **P. S. Stephanou\***, “On the consistent modeling of shear-thickening polymer solutions”, *Phys. Fluids* **33**, 063107 (2021). [Citations: 5].

30. **P. S. Stephanou\***, “Elucidating the rheological implications of adding drug-carrying particles in blood”, *Rheol. Acta* **60**, 603–616 (2021). [Citations: 2].

31. M. Papademetriou, and **P. S. Stephanou\***, “Modeling the rheological response of crude oil emulsions”, *Phys. Fluids*, **34**, 113107 (2022) [Citations: 3].

32. V. M. Nikiforidis, D. G. Tsakiris, and **P. S. Stephanou\***, “On the use of a non-constant non-affine or slip parameter in polymer rheology constitutive modeling”, *Dynamics*, **2**, 380–398 (2022) [invited, free-of-charge, Selected for Cover page, Citations: 2].

33. **P. S. Stephanou\***, P. Vafeas, and V. G. Mavrantzas, “Non-equilibrium thermodynamics modelling of the stress-strain relationship in soft two-phase elastic-viscoelastic materials”, *J. Non-Equilib. Thermodyn.* **48**, 91–105 (2023) [Citations: 2].

34. **P. S. Stephanou**, “Quantifying the oscillatory behavior in start-up shear by analytically solving the Johnson–Segalman/Gordon–Schowalter model”, *J. Non-Newt. Fluid Mech.* **312**, 104966 (2023) [invited, Citations: 0].

35. A. K. Ioannou, and **P. S. Stephanou\***, “Non-equilibrium thermodynamics modelling of the rheological response of cement pastes”, *J. Rheol.* **67**, 849 (2023). [Selected as Featured article and highlighted in *Scilight* 2023, 221109 (2023). Citations: 0].

36. P. C. Konstantinou, and **P. S. Stephanou\***, “Predicting high-density polyethylene melt rheology using a multimode tube model derived using non-equilibrium thermodynamics”, *Polymers*, **15**, 3322 (2023) [Open access, free-of-charge, Citations: 3].

37. M. Giakoumi, **P. S. Stephanou\***, K. Kapnisis\*, and A. Anayiotos, “On the Development of Physiologically Based Toxicokinetic Models (PBTK) for Cardiovascular Implants”, *Regulatory Toxicology and Pharmacology*, **144**, 105489 (2023). [Citations: 2].

38. **P. S. Stephanou\***, C. Georgantopoulos, A. Causa, and M. Wilhelm, “Modeling the Rheological Behavior of Silica Filled Rubber Compounds”, *Phys. Fluids*, **35**, 113332 (2023). [Selected as Editor’s pick article, Citations: 1]

39. M. Giakoumi, **P. S. Stephanou**, D. Kokkinidou, C. Papastefanou, A. Anayiotos, and K. Kapnisis\*, “A Predictive Toxicokinetic Model for Nickel Leaching from Vascular Stents”, *ACS Biomaterials Science & Engineering*, **10**, 2534–2551 (2024). [Citations: 0].

40. **P. S. Stephanou**, “Variable entanglement density constitutive rheological model for polymeric fluids”, *Rheol. Acta* **63**, 379–395 (2024). [Citations: 1].

41. **P. S. Stephanou**, “Inconsistency between the micropolar theory and non-equilibrium thermodynamics for polar fluids”, *J. Non-Equil. Thermo.* **49**, 335–346 (2024). [Citations: 0].

42. **P. S. Stephanou**, “A model with coupled Maxwell modes using Giesekus’ postulate”, *Phys. Fluids* **36**, 083109 (2024). [Citations: 0].

43. M. Giakoumi, K. Kapnisis, A. Anayiotos, and **P. S. Stephanou\***, “Analytical Solutions of PBTK Models for Evaluating the Impact of Surface Diffusion Characteristics on the Leaching Profile of Implant Bioproducts”, *Mathematical and Computational Applications*, **29**, 101 (2024). [Open access, Citations: 0].

44. M. Christodoulou, M. Kyriakou, **P. S. Stephanou**, and M. Koutinas\*, “Development of a hybrid gene regulatory network-bioprocess model to enhance the prediction of bioethanol production by *Saccharomyces cerevisiae*”, *Industrial & Engineering Chemistry Research*, accepted,

(2025).

45. P. Polykarpou, E. Kaliviotis, **P. S. Stephanou\***, “Modeling the shear-induced migration of rigid and deformable particles in a Newtonian suspending fluid”, *Phys. Fluids*, accepted (2025).

#### PUBLICATIONS SUBMITTED OR UNDER REVIEW (\* denotes the corresponding author)

46. F. Karami, and **P. S. Stephanou\***, “Considering a non-constant anisotropicity parameter in the Giesekus model”, *Polymers*, submitted (2025).

#### PUBLICATIONS UNDER PREPARATION (\* denotes the corresponding author)

1. F. Karami, and **P. S. Stephanou\***, “The Giesekus model revisited”, *J. Non-Newt. Fluid Mech.*, under preparation (2025).
2. P. Polykarpou, E. Kaliviotis, **P. S. Stephanou\***, “Modeling the shear-induced migration of rigid and deformable particles in power-law suspending fluids”, *Phys. Fluids*, under preparation (2025).
3. A. K. Ioannou, and **P. S. Stephanou\***, “A constitutive rheological model accurately addressing the rheological response of lunar regolith simulant and water pastes”, *CEAS Space Journal*, under preparation (2025).
4. A. K. Ioannou, and **P. S. Stephanou\***, “A constitutive model for cement pastes validated over a spectrum of temperature and water-to-cement ratio values”, *Rheol. Acta*, under preparation (2025).
5. M. Giakoumi, **P. S. Stephanou**, P. Mavri, A. Anayiotos, and K. Kapnisis\*, “Predictive Capability Testing and Sensitivity Analysis of Physiologically Based Toxicokinetic (PBTK) Models for Vascular Implants”, under preparation (2025).
6. M. M. Michail, K. P. Patsalidou, P. Polykarpou, E. Kaliviotis, **P. S. Stephanou\***, “A constitutive model addressing the Poisson distribution of rouleau sizes developed using non-equilibrium thermodynamics”, under preparation, *J. Rheol.* (2026).
7. K. Georgiou, A. Constantinou, **P. S. Stephanou\***, and N. Drousiotis, *Gas Science and Engineering*, under preparation (2026).
8. **P. S. Stephanou\***, D. G. Tsakiris, and V. G. Mavrantzas, “Complete rederivation of the Zimm model for an infinitely dilute solution of polymer rings in theta solvent and a rigorous test against detailed Molecular Dynamics simulation data”, under preparation (2026).
9. **P. S. Stephanou**, “Non-equilibrium thermodynamics modeling of chemically responsive polymer solutions”, *J. Rheol.*, under preparation (2026).

#### CITATIONS (until November 2024, based on Scopus database)

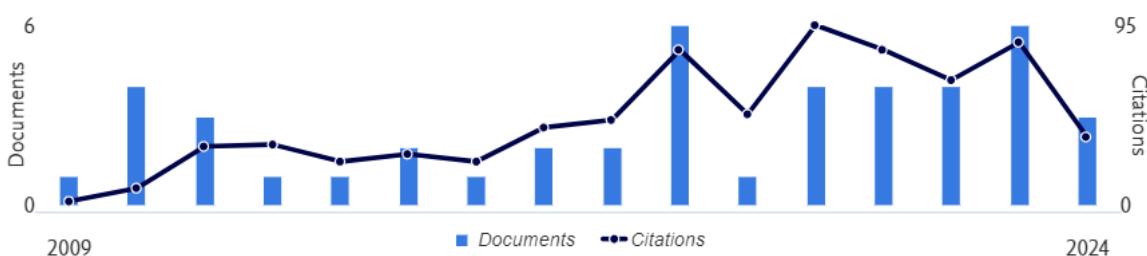
<https://www.scopus.com/authid/detail.uri?authorId=26032382500>

By others: 497 (65%)

Self-citations: 268 (35%)

Total: 765

Hirsch h index: 17 (11 when excluding self-citations)



#### BOOKS EDITED

1. P. S. Stephanou, « Lab Notes on Chemical Processes (CEN 210)», Cyprus University of Technology, 2019.
2. P. S. Stephanou, « Lab Notes on Unit Operations I (CEN 209E)», Cyprus University of Technology, 2020, 2021.

3. P. S. Stephanou, « Lab Notes on Unit Operations II (CEN 327E)», Cyprus University of Technology, **2020, 2021, 2022**.
4. P. S. Stephanou, « Lab Notes on Unit Operations (CEN 403)», Cyprus University of Technology, **2023, 2024**.

#### SPECIAL ISSUES EDITED

1. V.G. Mavrantzas, P. S. Stephanou (Guest Editors), Special Issue on: [Theory and Simulations of Entangled Polymers](#), Polymers, **2019**.
2. D. Tsalikis, P. S. Stephanou (Guest Editors), Special Issue on: [Topology and Dynamics of Ring Polymers](#), Polymers, **2021**.
3. P. S. Stephanou, C. Georgantopoulos, (Guest Editors), Special Issue on: [Rheological Properties of Polymer and Polymer Composites](#), Polymers, **2023-2024**.

#### BOOKLETS

1. [«Why become a Chemical Engineer»](#), (in Greek) prepared by P. S. Stephanou and uploaded on the DCE's webpage, **2020**.

#### OTHER PUBLICATIONS

1. «Τὰ πάντα ρέιν» (Everything flows), (in Greek) P. S. Stephanou, an article published in the Cyprus Scientific and Technical Chamber (ETEK) monthly newsletter, Vol 279, [pp. 24-25, July 2023](#).

#### 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, *6<sup>th</sup> 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, *7<sup>th</sup> 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<sup>th</sup> International Conference from Scientific Computing to Computational Engineering (4<sup>th</sup> 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 (10<sup>th</sup> 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 (10<sup>th</sup> 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”, *7<sup>th</sup> 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<sup>th</sup> 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, *9<sup>th</sup> 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. Tsaliakis, **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", *11th 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", *11th Panhellenic Chemical Engineers' Conference*, Thessaloniki, Greece, May 25-27 (2017) [in Greek].
14. **P. S. Stephanou**, D. G. Tsaliakis, 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", *11th 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<sup>h</sup> Panhellenic Chemical Engineers' Conference*, Thessaloniki, Greece, May 25-27 (2017).
16. **P. S. Stephanou**, D. G. Tsaliakis, 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* (2018) [Invited].
17. A. K. Ioannou, and **P. S. Stephanou**, "Modeling the rheological response of cement paste", *13<sup>th</sup> Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 2-4 (2022) [in Greek].
18. M. Papademetriou, and **P. S. Stephanou**, "Modeling the rheological response of crude oil", *13<sup>th</sup> Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 2-4 (2022) [in Greek].

## INVITED PRESENTATIONS

1. **P. S. Stephanou**, D. G. Tsaliakis, 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).
2. **P. S. Stephanou**, D. G. Tsaliakis, E. N. Skountzos and V. G. Mavrantzas, "Hierarchical Modelling and Simulation of the viscoelasticity of polymer melt nanocomposites: Non-Equilibrium Thermodynamics modeling coupled with Molecular Simulations", *12th Hellenic Polymer Society International Conference 2018*, Ioannina, Greece, September 30- October 3 (2018). [Prof. Mavrantzas invited, P.S.S. substituting].
3. **P. S. Stephanou** "The use of atomistic simulations to guide the derivation and verification of molecular theories", SimEA seminar series, Computation-based Science and Technology Research Center (CaSToRC), The Cyprus Institute (CyI), Nicosia, Cyprus, June 15 (2021) [taking place online due to Covid].
4. **P. S. Stephanou** "Modeling the rheological behavior of drilling fluids from a non-equilibrium thermodynamics perspective", Eastern Mediterranean Conference & Exhibition (EMC 2021), Nicosia, Cyprus, November 10-12 (2021). [it was scheduled to take place in 2020 but was rescheduled due to the Covid outbreak]
5. **P. S. Stephanou** "Non-equilibrium thermodynamics modeling of polymer nanocomposites", NANOMEC Workshop: "Computational Modeling of Heterogenous Materials: from atomistic to the Engineering scale", The Cyprus Institute (CyI), Cyprus, March 20-21 (2023).
6. **P. S. Stephanou** "A variable entanglement density constitutive model for entangled polymer systems from nonequilibrium thermodynamics: Comparison with atomistic steady-state NEMD simulation data", NANOMEC Workshop: "Computational Modelling of Molecular Systems:

from Atoms to the In-silico Design of Materials", The Cyprus Institute (CyI), Cyprus, May 20-21 (2024).

7. **P. S. Stephanou** "Use of non-equilibrium thermodynamics to derive a constitutive rheological model with a variable entanglement density", *39<sup>th</sup> Panhellenic Conference on Solid State Physics & Materials Science (FSK39)*, Paphos, Cyprus, September 14-17 (2025).

## PLENARY PRESENTATIONS

1. **P. S. Stephanou** "Non-equilibrium thermodynamics modeling of complex fluids: From polymer melts to cement pastes", *11<sup>th</sup> International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros, Greece, June 11 – 14 (2025) [plenary presentation as the first recipient of the "Tasos C. Papanastasiou Award" of HSR].

## PRESENTATIONS IN CONFERENCES/WORKSHOPS (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", *6<sup>th</sup> 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, *7<sup>th</sup> 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, *4<sup>th</sup> International Conference from Scientific Computing to Computational Engineering (4<sup>th</sup> 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", *6<sup>th</sup> 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", *6<sup>th</sup> 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", *7<sup>th</sup> 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<sup>th</sup> 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", *8<sup>th</sup> 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) *8<sup>th</sup> 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”, *9<sup>th</sup> 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), *9<sup>th</sup> 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”, *9<sup>th</sup> 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”, *7<sup>th</sup> 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”, *10<sup>th</sup> 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”, *7<sup>th</sup> 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”, *20<sup>th</sup> 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” *20<sup>th</sup> 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 modeling and atomistic simulation of polymer nanocomposites”, *11<sup>th</sup> 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), *11<sup>th</sup> 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), *11<sup>th</sup> 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”, *12<sup>th</sup> Annual European Rheology Conference (AERC 2017)*, Copenhagen, Denmark, April 3-6

(2017).

- 28. **P. S. Stephanou**, D. G. Tsaklis, 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. Tsaklis, 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*, 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), *11th 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”, *11th Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 25-27 (2017) [in Greek].
- 32. **P. S. Stephanou**, D. G. Tsaklis, 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”, *11th 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<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 25-27 (2017).
- 34. **P. S. Stephanou**, D. G. Tsaklis, 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).
- 38. **P. S. Stephanou**, “The unique position of Chemical Engineering at the interface between Physics and Engineering”, *1st Alumni Symposium of the Department of Chemical Engineering of the University of Patras*, Patras, Greece, 15-16 June (2018).
- 39. **P. S. Stephanou**, D. G. Tsaklis, E. N. Skountzos, and V. G. Mavrantzas, “A hierarchical approach to the rheology of polymer melt nanocomposites: non-equilibrium thermodynamics modeling coupled with atomistic molecular dynamics simulations”, *8th International Workshop and Summer School on Nonequilibrium Thermodynamics (IWNET 2018)*, Sint-Michielsgestel, The Netherlands, July 1-6 (2018).
- 40. D. G. Tsaklis, E. N. Skountzos, **P. S. Stephanou**, and V. G. Mavrantzas, “On the role of chain end-functional groups on microscopic structure and dynamics of polymer nanocomposites”, *European Polymer Congress (EPF) 2019*, Heraklion, Crete, Greece, 9-14 June (2019).
- 41. **P. S. Stephanou**, I. Ch. Tsimouri, G. C. Georgiou, and V. G. Mavrantzas, “Understanding the rheological behaviour of blood from a non-equilibrium thermodynamics perspective”, *9th International Meeting of the Hellenic Rheology Society (HSR 2019)*, Pythagoreion, Samos, Greece, 23-27 June (2019).
- 42. **E. N. Skountzos**, D. G. Tsaklis, **P. S. Stephanou**, and V. G. Mavrantzas, “Atomistic simulations combined with advanced modelling for the prediction of the microscopic dynamics

of polymer nanocomposites”, *5th Workshop for Graduates and Post-Docs in Chemical Engineering Sciences*, Patras, Greece, 6 November (2019) [Received the Best Oral presentation Award].

- 43. **K. Kapnisis, P. S. Stephanou**, D. Hadjiloizi, A. Afantitis, and A. Anayiotos. “Modeling Nickel Biotransport from Cardiovascular Stents”, *Summer Biomechanics, Bioengineering, and Biotransport (SB3C) Conference*, Vail, Colorado, USA, June 17 – 20, (2020).
- 44. E. N. Skountzos, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas “Coupling theory and simulations to fully elucidate the important role of end groups in poly(ethylene glycol) - silica nanocomposite melts”, *CORAL workshop on Complex Fluids in Manufacturing*, London UK, April 21 (2021) [taking place online due to Covid].
- 45. E. N. Skountzos, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas “A combined theoretical-simulation approach to microstructure and dynamics of poly(ethylene glycol) - silica nanocomposite melts”, *The first EUt Workshop on Nanomaterials and Nanotechnologies*, April 28-29 (2021) [taking place online due to Covid].
- 46. **P. S. Stephanou**, I. Ch. Tsimouri, and V. G. Mavrantzas, “A two-species model for the rheology of associative polymer solutions from nonequilibrium thermodynamics”, *92<sup>nd</sup> Annual Meeting of The Society of Rheology*, Bangor, Maine, USA, October 10-14 (2021) [online prerecorded talk due to Covid].
- 47. **P. S. Stephanou**, “Modelling the Rheological Behavior of Drilling Fluid from Non-Equilibrium Thermodynamics Perspectives”, *Eastern Mediterranean Conference (EMC 2021)*, Nicosia, Cyprus, November 10-12 (2021).
- 48. **T. S. Alexiou**, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas, “Conformation and dynamics of short linear and ring DNA molecules in the cross-over from the dilute to the semi-dilute solution regime: insights from atomistic molecular dynamics simulations” (poster), *13th Hellenic Polymer Society International Conference- POLYCONF 2021*, Athens, Greece, December 12-16 (2021). [Received the Best Poster presentation Award].
- 49. **V.-M. Nikiforidis**, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas, “On the relationship between stress and conformation tensors in state-of-the-art constitutive models for polymer melts and the possible additional role of chain tumbling” (poster), *Annual European Rheology Conference (AERC 2022)*, Sevilla, Spain, April 26-28 (2022).
- 50. **P.S Stephanou**, “Deriving a constitutive model for predicting the rheological response of drug-carrying particles”, *13<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Patras, Greece, June 2-4 (2022).
- 51. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the rheological response of cement paste”, *13<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Patras, Greece, June 2-4 (2022).
- 52. **M. Papademetriou**, and **P. S. Stephanou**, “Modeling the rheological response of crude oil”, *13<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Patras, Greece, June 2-4 (2022).
- 53. **M. Christodoulou**, M. Kyriakou, **P.S Stephanou**, M. Koutina, “Development of a Gene Regulatory model to enhance the prediction of bioethanol production by *saccharomyces cerevisiae*” (poster), *13<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Patras, Greece, June 2-4 (2022).
- 54. **P. S. Stephanou**, I. Ch. Tsimouri, and V. G. Mavrantzas, “A two-species model for the rheology of associative polymer networks from nonequilibrium thermodynamics”, *10<sup>th</sup> International Meeting of the Hellenic Society of Rheology*, Skiathos, Greece, June 29-July 2, (2022).
- 55. **P. S. Stephanou**, D. G. Tsalikis, C. Christopoulou, and V. G. Mavrantzas, “Introducing a variable entanglement density constitutive rheological model based on principles of non-equilibrium thermodynamics”, *Topology, Physics, and Chemistry of Soft Matter (Eutopia IV)*, Trento, Italy, September 5-9, (2022).
- 56. E. N. Skountzos, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas “A combined theoretical-simulation approach to microstructure and dynamics of poly(ethylene glycol) - silica nanocomposite melts”, *5th International Conference on Structural Nano Composites (NANOSTRU 2023)*, May 23-25 (2023).
- 57. **P. Konstantinou**, and **P. S. Stephanou**, “A generalized differential constitutive equation for polymer melts with a broad molecular weight distribution” (poster) *2<sup>nd</sup> International*

*Conference on Sustainable Chemical and Environmental Engineering (SUSTENG 2023), Limassol, Cyprus, June 14-18 (2023).*

- 58. M. Christodoulou, M. Kyriakou, **P. S. Stephanou**, M. Koutinas, “Improving prediction of bioethanol production through construction of a gene regulatory model in *Sccharomyces cerevisiae*” (poster) *2<sup>nd</sup> International Conference on Sustainable Chemical and Environmental Engineering (SUSTENG 2023)*, Limassol, Cyprus, June 14-18 (2023).
- 59. E. N. Skountzos, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas “A combined theoretical-simulation approach to microstructure and dynamics of poly(ethylene glycol) - silica nanocomposite melts”, *XIXth International Congress on Rheology (ICR 2023)*, July 29-August 4 (2023).
- 60. **P. S. Stephanou**, “Deriving a constitutive model for predicting the rheological response of drug-carrying particles” (poster), *XIXth International Congress on Rheology (ICR 2023)*, July 29-August 4 (2023).
- 61. **P. S. Stephanou**, D. G. Tsalikis, and V. G. Mavrantzas, “A variable entanglement density constitutive model for entangled polymer systems from nonequilibrium thermodynamics”, *Annual European Rheology Conference (AERC 2024)*, Leeds, UK, April 9-12 (2024).
- 62. E. N. Skountzos, D. G. Tsalikis, **P. S. Stephanou**, and V. G. Mavrantzas “A combined theoretical-simulation approach to microstructure and dynamics of poly(ethylene glycol) - silica nanocomposite melts”, *MecaNano’s 2<sup>nd</sup> General Meeting*, May 1-3 (2024).
- 63. **P. S. Stephanou** “Using nonequilibrium thermodynamics to derive a variable entanglement density constitutive model for entangled polymer systems: Comparison with atomistic steady-state NEMD simulation data”, *3<sup>rd</sup> EUt+ Workshop on Nanomaterials and Nanotechnologies (EUTINN) workshop*, May 20-21 (2024) [presenting online].
- 64. **P. Polykarpou**, **P. S. Stephanou**, and E. Kaliviotis, “Modeling the shear-induced migration of Red Blood Cells under physiological conditions”, *14<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 29-31 (2024).
- 65. M. Giakoumi, **P. S. Stephanou**, K. Kapnisis, and A. Anayiotos, “Incorporating confidence intervals in physiologically based toxicokinetic (PBTK) modeling”, *14<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 29-31 (2024).
- 66. M. Christodoulou, M. Kyriakou, **P. S. Stephanou**, and M. Koutinas, “Development of a Gene Regulatory Model to enhance prediction accuracy of Bioethanol fermentation by *Saccharomyces Cerevisiae*”, *14<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 29-31 (2024).
- 67. K. Georgiou, A. Constantinou, **P. S. Stephanou**, and N. Drousiotis, “Optimized in silico sour gas processing for offshore deepwater gas technology applications at in the Eastern Mediterranean region” (poster), *14<sup>th</sup> Panhellenic Chemical Engineers’ Conference*, Thessaloniki, Greece, May 29-31 (2024).
- 68. K. Georgiou, A. Constantinou, **P. S. Stephanou**, and N. Drousiotis, “Optimized in silico sour gas processing for offshore deepwater gas technology applications at in the Eastern Mediterranean region” (poster), *1<sup>st</sup> Conference of the Cyprus Advanced Materials Network (Cy-AMN)*, Nicosia, Cyprus, January 13-14 (2025).
- 69. **P. Polykarpou**, **P. S. Stephanou**, and E. Kaliviotis, “Modeling the shear-induced migration of Red Blood Cells under physiological conditions”, (poster) *1<sup>st</sup> Conference of the Cyprus Advanced Materials Network (Cy-AMN)*, Nicosia, Cyprus, January 13-14 (2025).
- 70. A. K. Ioannou, and **P. S. Stephanou**, “Modeling the rheological response of cement paste”, (poster) *1<sup>st</sup> Conference of the Cyprus Advanced Materials Network (Cy-AMN)*, Nicosia, Cyprus, January 13-14 (2025).
- 71. **P. S. Stephanou** “Considering a variable entanglement density in constitutive modeling of entangled polymer melts using non-equilibrium thermodynamics”, *1<sup>st</sup> Conference of the Cyprus Advanced Materials Network (Cy-AMN)*, Nicosia, Cyprus, January 13-14 (2025).
- 72. **P. Polykarpou**, **P. S. Stephanou**, and E. Kaliviotis, “Modelling the shear-induced migration of rigid and deformable particles in Newtonian or non-Newtonian fluids”, *1<sup>st</sup> Cyprus Rheology and Fluidics Technology Centre (CraFTC) Research-Academic Workshop*, Limassol, Cyprus, February 6 (2025).
- 73. **P. Polykarpou**, **P. S. Stephanou**, and E. Kaliviotis, “Modeling of the shear-induced migration

of red blood cells in Newtonian and non-Newtonian fluids”, *4<sup>th</sup> Doctoral Colloquium Cyprus 2025*, Limassol, Cyprus, April 5 (2025).

- 74. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the rheological response of cement paste”, *4<sup>th</sup> Doctoral Colloquium Cyprus 2025*, Limassol, Cyprus, April 5 (2025).
- 75. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the rheological response of cement paste”, *4<sup>th</sup> Doctoral Colloquium Cyprus 2025*, Limassol, Cyprus, April 5 (2025).
- 76. **P. S. Stephanou** “A variable entanglement density constitutive model for entangled polymer melts derived using non-equilibrium thermodynamics and comparison with atomistic NEMD simulations”, *10th International Workshop on Nonequilibrium Thermodynamics (IWNET 2025)*, Syros, Greece, June 8 – 11 (2025).
- 77. **P. Polykarpou**, E. Kaliviotis, and **P. S. Stephanou**, “Modeling the shear-induced migration of red blood cells in Newtonian and non-Newtonian fluids”, *11<sup>th</sup> International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros, Greece, June 11 – 14 (2025)
- 78. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the Rheological Behavior of Cement Pastes”, (poster), *11<sup>th</sup> International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros, Greece, June 11 – 14 (2025)
- 79. **M. M. Michail**, **K. P. Patsalidou**, P. Polykarpou, E. Kaliviotis, and **P. S. Stephanou**, “A constitutive hemorheological model addressing the aggregation of red blood cells at low hematocrit values”, (poster) *11<sup>th</sup> International Meeting of the Hellenic Society of Rheology (HSR 2025)*, Syros, Greece, June 11 – 14 (2025).
- 80. **P. Polykarpou**, E. Kaliviotis, and **P. S. Stephanou**, “Modeling microscale blood flow, influenced by the shear-induced migration of deformable cells”, *9<sup>th</sup> International Conference on Micro and Nano Flows (MNF 2025)*, Edinburgh, Scotland, UK, September 3-5 (2025).
- 81. **P. Polykarpou**, E. Kaliviotis, and **P. S. Stephanou**, “Modelling of the shear-induced migration of rigid and deformable particles in Newtonian and non-Newtonian fluids”, *39<sup>th</sup> Panhellenic Conference on Solid State Physics & Materials Science (FSK39)*, Paphos, Cyprus, September 14-17 (2025).
- 82. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the Rheological Behavior of Cement Pastes over a spectrum of temperature and water-to-cement ratio”, *39<sup>th</sup> Panhellenic Conference on Solid State Physics & Materials Science (FSK39)*, Paphos, Cyprus, September 14-17 (2025).

## 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. Tsakalis, 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, Limassol, 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].
10. **P. S. Stephanou**, I. Ch. Tsimouri, and V. G. Mavrantzas, “A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics”, Department of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology, Limassol, Cyprus, March 2 (2018) [in Greek].
11. **P. S. Stephanou**, I. Ch. Tsimouri, and V. G. Mavrantzas, “A constitutive rheological model for agglomerating blood derived from nonequilibrium thermodynamics”, Department of Mathematics and Statistics, University of Cyprus, Nicosia, Cyprus, March 28 (2018) [in Greek].
12. **P. S. Stephanou** “Modeling the flow and deformation of complex systems with the use of non-equilibrium thermodynamics”, Department of Environmental Science and Technology, Cyprus University of Technology, Limassol, Cyprus, October 17 (2018). [in Greek].
13. **P. S. Stephanou** “Modeling the flow and deformation of complex systems with the use of non-equilibrium thermodynamics”, Department of Mechanical and Manufacturing Engineering, University of Cyprus, Nicosia, Cyprus, January 7 (2019). [in Greek].
14. **P. S. Stephanou** “Development of scale-bridging methodologies to model complex fluids”, Department of Chemical Engineering, Cyprus University of Technology, Limassol, Cyprus, November 12 (2019). [in Greek].
15. **P. S. Stephanou** “Understanding the phase behavior and microstructure of polymer nanocomposites: A combined theoretical-simulation approach”, Institute for Chemical Technology and Polymer Chemistry (ITCP), Polymer Materials Group of Prof. Dr. M. Wilhelm, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany, February 2 (2022). [taking place online].
16. **P. Polykarpou, P. S. Stephanou**, and E. Kaliviotis, “Modeling the shear-induced migration of deformable Red Blood Cells under physiological conditions”, (poster) *Cyprus Scientific and Technical Chamber (ETEK) meeting “Engineers and their Role in Research and Innovation”*, Nicosia, Cyprus, May 22 (2025).
17. **A. K. Ioannou**, and **P. S. Stephanou**, “Modeling the rheological response of cement paste”, (poster) *Cyprus Scientific and Technical Chamber (ETEK) meeting “Engineers and their Role in Research and Innovation”*, Nicosia, Cyprus, May 22 (2025).

#### **ADVISEMENT AS ASSO. PROFESSOR AT THE DEPARTMENT OF CHEMICAL ENGINEERING, CUT**

##### Undergraduate students

1. Matthaios Giakoumi, Topic: Development of a new physiologically based toxicokinetic (PBTK) model (between 03/2020-06/2021 graduated in July 2021, co-advancement with Prof. A. Anayiotis and Dr. K. Kapnisis at DLEMSE, CUT). [Now a PhD student at Hildebrand Department of Petroleum and Geosystems Engineering, The University of Texas at Austin, TX, USA]
2. Amalia Ioannou, Topic: Modeling the rheological behavior of cement pastes (between 05/2021-05/2022, graduated in July 2022). Amalia's thesis received the award of the best degree thesis in 2022, was published in the *Journal of Rheology*, was selected as a Featured article by the Editor-in-Chief, and highlighted in [Scilight 2023, 221109 \(2023\)](#) [Now PhD student at DCE, CUT].
3. Maria Papadimitriou, Topic: Modeling the rheological behavior of crude oil (between 05/2021-05/2022, graduated in June 2023). [Now at Alambra Dairies Ltd, Larnaka, Cyprus]

4. Neofyta Kyriakidou, Topic: CFD modeling of heat distribution in ovens (between **05/2024-05/2025**, graduated in June **2025**).
5. Marianna Michail, Topic: Modeling the rouleaux size distribution (between **05/2025-05/2026**, graduated in June **2026**).
6. Maria Gregoriou, Topic: 3D simulations of cement paste (between **05/2025-05/2026**, graduated in June **2026**).
7. Maria Soulaki, Topic: Modeling the rheological response of polymer melts (between **05/2025-05/2026**).
8. Anthia Aresti, Topic: Modeling the rheological behavior of mayonnaise (between **05/2025-05/2026**).

#### MSc students

1. Demetris Vrakas, Topic: Mathematical and Computational Modeling of Metal Ion Release from Cardiovascular Implants (tentative title) (between **01/2023-Today**, co-advisement with Dr. K. Kapnisis at c.)

#### PhD students

1. Pavlina Konstantinou, Topic: Modeling the rheology of entangled polymers (between **01/2023-08/2023** when she terminated her PhD studies).
2. Kyproula Georgiou, Topic: Optimized in silico sour gas processing for offshore deepwater gas technology applications (between **09/2023-Today**, co-advisement with Assos. Prof. Ach. Constantinou at DCE, CUT, funded by research grant SUGARS).
3. Panayiota Polykarpou, Topic: Modeling of shear-induced migration of red blood cells (between **01/2024-Today**, co-advisement with Assos. Prof. Efstathios Kaliviotis, DMEMSE, CUT, funded by research grant CRaFTC).
4. Amalia Ioannou, Topic: Optimizing the extraterrestrial 3D printing of cement-based structures (between **09/2024-Today**, funded by ESA's research grant ID: I-2023-10808).

#### Post-Doctoral Collaborators

1. Dr. Terpsichori (Chara) S. Alexiou, Topic: Performing atomistic NEMD simulations to calculate an asymmetric stress tensor (**09/2021-10/2021**) [Now Postdoctoral Researcher, Faculty of Physics, University of Vienna, Austria]
2. Dr. Vasileios-Martin Nikiforidis Topic: Performing atomistic NEMD simulations to calculate an asymmetric stress tensor (**11/2021-04/2022**).
3. Dr. Marios Kosta, Topic: Non-equilibrium thermodynamics modeling of the rheological response of miscible entangled polymer blends (**08/2022-08/2023**). [Now Special Teaching Staff at DMEMSE, CUT].

### **MEMBER OF DEGREE THESIS EXAMINATION COMMITTEES**

1. **2021**: Eleana Xarkou, Konstantina Stylianou, Nikolas Kantzas, Xristina Panagiotou (Total 4).
2. **2022**: Panagiota Efraim, Xristina Kyriakou, Anastasia Spanou, Georgia Paschalidou, Natassa Karetou, Imat Kouti, Styliani Iakovou (Total 7).
3. **2023**: Evgenia Christofi, Christina Christofidou, Pantelitsa Christou, Aliki Christodoulou (Total 4).
4. **2024**: Konstantinos Achillidis, Antonis Prokopiou, Despoina Konstantinou, Eleni Ilia, Styliani Piripitsi (Total 5).
5. **2025**: Georgia Alekou, Charalampos Christodoulou, Antreas Michail, Mary Patsalou, George Mouskis, Athina Karakosta (Total 6).

### **MEMBER OF MSc THESIS EXAMINATION COMMITTEES**

1. Michalis Xrysostomou, "Blood Fluid Mechanics and Rheology – Study of the effect of cardiovascular implants on Blood Fluid Mechanics" DMEMSE, CUT (**June 4<sup>th</sup> 2022**) (3-member committee, acting as head of the committee; advisor: Assos. Prof. Efstathios Kaliviotis, DMEMSE, CUT).

### **ADVISORY COMMITTEE MEMBER OF PhD STUDENTS**

1. Despoina Konstantinou "Production of hydrogen using zero-valent iron in anaerobic digestion" (Date of comprehensive examination: February 12<sup>th</sup> 2024).
2. Panayiota Adamou "Catalytic Decomposition of Hydrous Hydrazine into H<sub>2</sub> in a batch reactor" (Date of comprehensive examination: February 21<sup>st</sup> 2024).
3. Fryni Pyrilli "Development of bioprocesses for the biodegradation of bioplastics using algal-microbial co-cultures" (Date of comprehensive examination: May 26<sup>th</sup> 2025).
4. Rena Konstantinou "Development of bioprocesses for the biodegradation of bioplastics using polysaccharides" (Date of comprehensive examination: May 26<sup>th</sup> 2025).

#### **EXTERNAL MEMBER OF PhD EXAMINATION COMMITTEES**

1. Emmanuel-Theodoros Skountzos, "Molecular Simulation of Nanoparticle-based Systems: from their Agglomeration in Gas Phase to the Dynamic and Mechanical Properties of Polymer Nanocomposites" Department of Chemical Engineering, University of Patras, Greece (**April 15<sup>th</sup>, 2022**) [Now Research Assistant at NASA] (7-member committee)
2. Panayiotis Alatas, "Calculation of multi-time correlation functions in dissipative quantum  $\phi^4$  theory" Department of Chemical Engineering, University of Patras, Greece (**May 4<sup>th</sup>, 2023**). (7-member committee).
3. Nikolaos Patsalidis, "Multi-Scale Computational Modeling of Nanostructured Materials" CaSToRC, The Cyprus Institute, Cyprus (**November 13<sup>th</sup>, 2025**). (5-member committee).
4. Diego Chaparro, "Computational modeling of engineered nanosilver for biomedical applications" Department of Chemical Engineering, School of Chemical and Biomedical Engineering, The University of Melbourne, Melbourne, Australia (**January 2025**) (no viva or defense thesis presentation required; I assessed the thesis of the candidate).
5. Despoina Kokkinidou, "In vitro and in vivo study of the effect of cardiovascular stenting in hemodynamic, hematological and hemorheological parameters" DMEMSE, CUT (date not yet scheduled) (3-member committee, acting as head of the committee; advisor: Assos. Prof. Efstathios Kaliviotis, DMEMSE, CUT).

#### **STUDENT CO-ADVICE AS GRADUATE STUDENT**

##### Master Thesis students

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

#### **STUDENTS CO-ADVICE AS POST-DOCTORAL RESEARCHER**

##### Master Thesis students

1. Ioanna Tsimouri (academic advisor: Prof. V.G. Mavrantzas, graduated in **2018**) [Now Dr. Ioanna Tsimouri, Application Engineer, at Helmut Fischer, Cham, Zug, Switzerland]

##### Diploma Thesis students

1. Ioanna Tsimouri (academic advisor: Prof. V. G. Mavrantzas, graduated in **2016**).
2. Christos Georgantopoulos (academic advisor: Prof. V. G. Mavrantzas, graduated in **2018**). [Now Dr. Christos Georgantopoulos, Technical Service Manager - Polymers, at Omya, Oftringen, Aargau, Switzerland]

#### **ADMINISTRATIVE DUTIES**

1. Departmental Committee of Undergraduate Studies, 01/2021-today.
2. Departmental Committee of Postgraduate Studies, 05/2022-today.
3. Elected Cyprus University of Technology Senate member, 01/2022-12/2023 (2-year term).
4. Member of the Faculty Board, Faculty of Geotechnical Sciences and Environmental Management, 01/2023-today (2-year term).
5. Elected Department Vise-Head, 12/2024-11/2027 (3-year term).

#### **EVALUATOR FOR RESEARCH PROPOSALS**

Evaluator for research proposals submitted for funding in

1. Chilean National Science and Technology Commission (CONICYT), Government of Chile (July 2018: 1 proposal).

2. Hellenic Foundation for Research & Innovation (HFRI), Hellenic Republic (March 2019: 1 proposal).
3. Dutch Research Council (NWO), The Netherlands, [www.nwo.nl/aes](http://www.nwo.nl/aes) (July 2022: 1 proposal).

### **EVALUATOR FOR RECOGNITION OF QUALIFICATION**

Evaluator for qualifications of degrees in Chemical Engineering

1. The Cyprus Council of Recognition of Higher Education Qualifications (KY.S.A.T.S.), **2020-2025 (Annual appointments)**.

### **INVOLVEMENT IN COMMITTEES**

1. Invited by the Scientific Technical Chamber of Cyprus (ETEK) to participate in the action CYS/TC 26 "Circular Plastic Products" of the Cyprus Organization for Standardization (CYS) in the framework of standardization actions for the implementation of the National Circular Economy Action Plan, **04/2022-Today**
2. Invited by the Scientific Technical Chamber of Cyprus (ETEK) to participate in its Chemical Engineering Committee, where I have been selected to be the Head of this committee, **09/2024-Today** (3-year term)

### **REVIEWER FOR BOOKS**

1. Invited by the Cambridge University Press to proofread and edit the 1<sup>st</sup> edition of the textbook "A Modern Course in Transport Phenomena" by David C. Venerus and Hans Christian Öttinger, **2017**.

### **REVIEWER FOR SCIENTIFIC JOURNALS**

Reviewer for manuscripts submitted (the year denotes the time of my Reviewer activities) for consideration for publication in the following journals (also included the impact factor of 2021-2022):

1. Nature Communications, 2024 (I.F. 16.6)
2. Physical Review X (PRX), 2023 (I.F. 12.5).
3. Physical Review Letters (PRL), 2015,2024 (I.F. 8.6).
4. ACS Macro Letter, 2020 (I.F. 5.8)
5. Macromolecules, 2021-2022 (I.F. 5.7)
6. International Journal of Molecular Sciences 2023 (I.F. 5.6)
7. Nanomaterials (MDPI), 2023 (I.F. 5.3)
8. Powder Technology 2015 (I.F. 5.2).
9. Polymers (MDPI), 2019-2022 (I.F. 5.0).
10. Physics of Fluids, 2017-2025 (I.F. 4.6).
11. Scientific Reports, 2020-2021, 2024 (I.F. 4.9).
12. Journal of Chemical Physics, 2015 (I.F. 4.4).
13. Industrial and Engineering Chemistry Research, 2014-2015 (I.F. 4.1).
14. Annals of the New York Academy of Sciences 2025 (I.F. of 2023: 4.1).
15. Langmuir, 2013 (I.F. of 2020 3.8).
16. Frontiers in Physics, 2020-2021 (I.F. of 3.8).
17. Applied Physics Letters, 2021 (I.F. 3.7).
18. Soft Matter, 2013-2022 (I.F. 3.4).
19. Journal of Rheology, 2015-2025 (I.F. 3.3).
20. Energies (MDPI), 2020 (I.F. 3.2).
21. Polymer Engineering and Science, 2023 (I.F. 3.2).
22. Journal of Non-Newtonian Fluid Mechanics, 2012 (I.F. 3.1).
23. Chemical Physics Letters, 2016, 2019 (I.F. 2.8).
24. Entropy (MDPI), 2020-2022,2024 (I.F. 2.7).
25. Physical Review E (PRE), 2015-2017 (I.F. 2.4).
26. Colloids and Interfaces (MDPI), 2023 (I.F. 2.4)
27. Mathematics (MDPI), 2020-2021 (I.F. 2.4).
28. Rheologica Acta, 2022-2023 (I.F. 2.3).
29. Applied Rheology, 2020-2024 (I.F. 1.8).

30. Macromolecular Theory and Simulation, 2015 (I.F. 1.4).

## REVIEWER HONORS AND AWARDS

- Top Reviewer in 2023, The Journal of Rheology.
- Top Reviewer in 2024, The Journal of Rheology.

## CONFERENCE ACTIVITIES

1. Member of the Scientific Committee, *13<sup>th</sup> Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 2-4 (**2022**).
2. Session Chairing between 09:45-11:45 on Saturday, June 4, *13<sup>th</sup> Panhellenic Chemical Engineers' Conference*, Patras, Greece, June 2-4 (**2022**).
3. Session Chairing between 14:00-15:40 on Thursday, June 30, *10<sup>th</sup> International Meeting of the Hellenic Society of Rheology*, Skiathos, Greece, June 29-July 2 (**2022**).
4. Session Chairing between 09:00-10:00 on Thursday, September 8, *Topology, Physics, and Chemistry of Soft Matter (Eutopia IV)*, Trento, Italy, September 5-9, (**2022**)
5. Session Chairing between 09:00-10:20 on Friday, August 4, *XIXth International Congress on Rheology (ICR 2023)*, July 29-August 4 (**2023**).
6. Session Chairing between 08:50-10:10 on Friday, April 12, *Annual European Rheology Conference (AERC 2024)*, April 10-12 (**2024**).
7. Session Chairing between 09:45-11:00 on Friday, May 31, *14<sup>th</sup> Panhellenic Chemical Engineers' Conference*, May 29-31 (**2024**).
8. Session Chairing between 15:40-17:00 on Monday, June 9, *10<sup>th</sup> International Workshop on Nonequilibrium Thermodynamics (IWNET 2025)*, Syros, Greece, June 8 – 11 (**2025**).

## ORGANIZATION OF SCIENTIFIC MEETINGS

1. Assistance Personnel, *4<sup>th</sup> International Workshop on Non-Equilibrium Thermodynamics and Complex Fluids (IWNET)*, Rhodes, Greece, September 4-7, **2006**.
2. Assistance Personnel, *15<sup>th</sup> International Workshop of Numerical Methods for Non-Newtonian Flows*, Rhodes, Greece, June 14-17, **2007**.
3. Organizing Committee, *1st Workshop of the Cypriot Advanced Materials Network (Cy-AMN)*, Nicosia, Cyprus, January 13-14, **2025**.
4. Organizing Committee, *12<sup>th</sup> International Meeting of the Hellenic Society of Rheology (HSR 2028)*, Larnaka, Cyprus, July, **2028**.

## REFERENCES

Prof. Vlasis G. Mavrantzas Karatheodoris 1 Department of Chemical Engineering University of Patras Patras, GR 26504 Greece e-mail: <a href="mailto:vlasis@chemeng.upatras.gr">vlasis@chemeng.upatras.gr</a> tel.: (+30)-2610-997-398 fax: (+30)-2610-965-223 & Department of Mechanical Engineering ETH-Zürich Sonneggstrasse 3 Zürich, 8093 Switzerland e-mail: <a href="mailto:vlasios.mavrantzas@mat.ethz.ch">vlasios.mavrantzas@mat.ethz.ch</a> tel.: (+41)- 44 632 85 03	Prof. John Tsamopoulos Karatheodoris 1 Department of Chemical Engineering University of Patras Patras, GR 26504 Greece e-mail: <a href="mailto:tsamo@chemeng.upatras.gr">tsamo@chemeng.upatras.gr</a> tel.: (+30)-2610-997-203 fax: (+30)-2610-993-255
Prof. Antony N. Beris Department of Chemical and Biomolecular Engineering	Prof. Brian J. Edwards Department of Chemical & Biological Engineering

University of Delaware  
Newark, DE 19716  
USA  
tel.: (+1)-302-831-4416  
e-mail: [beris@che.udel.edu](mailto:beris@che.udel.edu)  
fax : (+1)-302-831-1048

Prof. Georgios C. Georgiou  
Department of Mathematics and Statistics  
Cyprus Oceanography Center  
University of Cyprus  
PO Box 20537  
1678 Nicosia, Cyprus  
e-mail: [georgios@ucy.ac.cy](mailto:georgios@ucy.ac.cy)  
tel.: (+357)-22-892612  
fax : (+357)-22-892601

Prof. Martin Kröger  
Department of Materials  
Institut f. Polymere, HCP F48.2  
ETH Zürich  
Leopold-Ruzicka-Weg 4  
8093 Zürich  
e-mail: [mk@mat.ethz.ch](mailto:mk@mat.ethz.ch)  
tel.: (+41)-44-632- 6622  
fax : (+41)-44-632-1076

University of Tennessee  
Knoxville, TN 37996-2200  
USA  
tel.: (+1)-302-865-9749596  
e-mail: [bjedwards@chem.engr.utk.edu](mailto:bjedwards@chem.engr.utk.edu)  
fax: (+1)-302-865-9747076

Prof. Emer. Hans Christian Öttinger  
Department of Materials  
Institut f. Polymere, HCP F47.2  
ETH Zürich  
Leopold-Ruzicka-Weg 4  
8093 Zürich  
e-mail: [hco@mat.ethz.ch](mailto:hco@mat.ethz.ch)  
tel.: (+41)-44-632-4633  
fax : (+41)-44-632-1076