PPS Newsletter

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April 2008 *Information to Polymer Processing Society Members*

PPS-24 in Salerno, Italy, the biggest to date?

The beautiful and historic city of Salerno, Italy, is situated 60 km south of Naples and offers an enchanting view of the scenery of the Gulf of Salerno facing the magnificent Amalfi Coast. Nearby are the ancient sites of Pompei and Paestum. Salerno has escaped mass tourism, and it is "authentically Italian", with a historic center, an ancient castle overlooking the city and the bay, and a long seafront promenade. Its marvelous year-round climate makes it possible to enjoy a "typical Italian" outdoor lifestyle. It will be the location of the PPS-24 annual meeting of the Polymer Processing Society (http://www.pps-24.com). The meeting will take place in June 15-19, 2008. The venue will be the Grand Hotel Salerno right on the coast overlooking Salerno Bay. Around 1200 submissions for papers to present have been received from more than 40 countries from around the world, making it perhaps the biggest annual meeting ever of the PPS. The team of Prof. Giuseppe Titomanlio is working very hard to make this meeting a grand success.

Map of Naples and Salerno Bays. Salerno, the site of PPS-24, is located near the Amalfi Coast (green arrow) and boasts many historical sites nearby (Pompei, Herculaneum, Paestum, etc).

One of the attractions of Salerno is the beautiful promenade near the Hotel and Conference Center.

Grand Hotel Salerno, the venue for the PPS-24 Annual Meeting, overlooking Salerno Bay.

Americas Regional Meeting PPS-2008 to be held in October in Charleston, South Carolina, USA

The Americas Regional Meeting PPS-2008 will be held in Charleston, South Carolina, USA. The meeting will take place in October 26-29, 2008 at the Francis Marion Hotel in the heart of historic Charleston. Charleston is well-known for its unique culture, which blends West African, traditional southern American and French elements. The technical program covers all important polymer processing sessions for which PPS is well known. More information can be found at http://caeff.ces.clemson.edu/pps2008. Special thanks are due to Profs. Douglas Hirt and Amod Ogale for all the hard work they are putting to make this a successful event.

Map of Charleston, SC, USA, with its waterfront, site of the Americas Regional Meeting 2008 of the PPS.


Typical colonial architecture of down-town Charleston, with the Charleston Museum being the first in the Americas.


Facilities in the CAEFF (Center for Advanced Engineering Fibers and Films) at Clemson University, the Organizers of the Americas-RM PPS-2008 Meeting.

Future Meetings

In its continuing effort to be a truly international society, PPS strives to have meetings every year in different parts of the world. The following list of upcoming meetings is a good indication of these efforts.

2008 Meetings

Americas Regional Meeting 2008, Charleston, South Carolina, USA, October 26-29, 2008 (http://caeff.ces.clemson.edu/pps2008/index.php/). Conference Chair: Profs. Hirt, Ogale

2009 Meetings

Annual Meeting PPS-25, Goa, India – March 1-5, 2009 (http://www.pps-25.com). Conference Chair: Prof. Ashok Misra

2010 Meetings

Annual Meeting PPS-26, Calgary, Canada – July 4-7, 2010 (http://www.pps-25.com). Conference Chair: Prof. Sundararaj

Two Morand Lambla Award Winners for 2008!

2008 is the year of two winners of the prestigious MORAND LAMBLA award of the PPS. The Committee decided to make two awards due to the closeness of the scores of the two outstanding winners. They are (in alphabetical order) *Patrick ANDERSON* from the Netherlands, and *Shih-Jung LIU* from Taiwan.

Patrick ANDERSON is Associate Professor of Fluid Mechanics in Polymer Processing at the Eindhoven University of Technology (TU/e) in the Netherlands. He studied Applied Mathematics at TU/e with Prof. Arnold Reusken. In 1999 he completed his Ph.D. degree from the Department of Mechanical Engineering at TU/e with Prof. Han Meijer. His PhD work was on distributive mixing of polymer melts and solutions using combined computational and theoretical methods. Following a break at Océ Technologies, working on hot-melt inkjet printing, he joined the Polymer Technology group at TU/e.

He is a member of PPS since 1997 and has attended more than 10 international or regional PPS meetings. At two meetings, in Yokohama and Athens, he was given the opportunity to present a keynote lecture and also a plenary lecture in Guimarães. In addition, he has acted as session organizer at several recent PPS meetings. The research interest of Patrick Anderson include structure development during flow, interfacial phenomena, microfluidics, mixing and polymer processing. Key topics are:

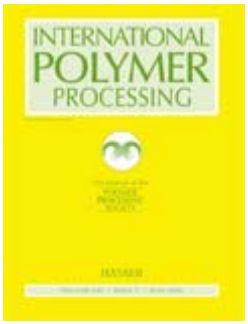
- the development of novel numerical methods to analyze distributive mixing in both static and dynamic mixers. In particular, the mapping method has proven to be powerful in optimization of mixing processes, and is finding new applications in the field of microfluidics;
- the extension of boundary integral models to describe the dynamics of viscous drops in confined flow. This approach is able to tackle the complex process of viscous drop coalescence over the complete range of length scales, i.e. about five orders. Also the effect of surfactants on drop deformation and breakup in shear flow has been unraveled, and their role has been summarized so that the outcome becomes accessible to the scientific and industrial community.
- the development and application of diffuse-interface models to predict the morphology and rheology of polymer blends. In addition, this type of modelling is applied to describe polymer phase separation in complex flow.

Shih-Jung LIU is Professor of Mechanical Engineering at Chang Gung University (CGU), Taiwan. He completed his PhD on modeling and simulation of part warpage in injection molding at the University of Wisconsin-Madison, USA, in 1992. After one year's research at McMaster University of Canada, Dr. Liu joined the Polymer Rheology and Processing Laboratory at the CGU since 1993, and has been involved in pioneering work on the concepts of various polymer processing techniques.

Dr. Liu's research work deals with theoretical and experimental processing of various polymeric materials. He is worldwide known for the development of water-assisted injection molding systems and significant accomplishments in gas-assisted injection molding. He is also recognized for his works in precision molding, rotational molding, ultrasonic/hot plate welding, thermoforming and blow molding of various plastics, and the processing of biodegradable polymers.

Dr. Liu has delivered invited/keynote lectures at various international conferences and has been a frequent invited lecturer at various universities and industrial companies in Taiwan. He is the author of more than 200 scientific publications including 90 journal papers, editor and co-editor of 6 books and the author of 12 patents. He is also serving as the Editor for Asia and Australia for the *Journal of Polymer Engineering (JPE)* and serves in the Editorial Board for the Journals of *Plastic, Rubber and Composites: Macromolecular Engineering (PRC-ME)* and *International Polymer Processing (IPP)*.

IPP Journal New Special Issues



The PPS Journal "International Polymer Processing" (IPP) continues its pursuit of excellence increasing publishing to 5 issues/year. Previous issues are now on-line at http://www.polymer-process.com. To download papers from this site, use your PPS membership number. In response to PPS member requests, papers in IPP will now have a DOI number, as well as a Hanser document number, which allows quick access to a paper for the on-line journal website.

PPS members are encouraged to have their university, company or research institute get an institutional subscription to International Polymer Processing. An institutional subscription allows non-PPS members to have access to the society's journal broadening the exposure of the journal. A brochure with ordering information is attached.

Other Meetings of Interest to PPS Members

ANTEC SPE, MAY 4-8, 2008, MILWAUKEE, WISCONSIN, USA
For information visit: **www.4spe.org**

XVth INTERNATIONAL CONGRESS ON RHEOLOGY
AUGUST 3-8, 2008, MONTEREY, CA, USA
For information visit: **http://www.rheology.org/ICR2008/**

17th International Conference on Composite Materials (ICCM17)
JULY 27-31, 2009, EDINBURGH, UK
For information visit:
https://www.eventsforce.net/iom/frontend/reg/tOtherPage.csp?pageID=1175&eventID=7&eventID=7

International Symposium on Mixing in Industrial Processes VI
August 17-21, 2008, Niagara Falls, Canada
For information visit: **http://www.ismip6.org/**

8th World Congress of Chemical Engineering (with several sessions on Polymer Processing and Green Polymers)
August 23-27, 2008, Montreal, Quebec, Canada
For information visit: **http://www.wccce8.org/**

International Society of Coating Science and Technology 14th Annual Symposium
September 7-10, 2008, Marina del Rey, California USA

For information visit: **http://www.iscst.org/**

SPE EUROTEC Conference
September 29 - October 3, 2009, BARCELONA, SPAIN
For information visit: **http://www.speeurope.org**

PPS Membership Website

A complete list of all PPS members, their addresses, phone numbers and e-mails, is available at the PPS membership website: http://pps.mcmaster.ca.
The user ID is "ppsmember" and the password "ppsmember".

Next Newsletter – November 2008

If you have comments on how to improve this newsletter or want to share some information in the next one, please contact the Newsletter Editor Prof. Evan Mitsoulis at mitsouli@metal.ntua.gr. The next issue of the Newsletter is due in November 2008.

Papers of General Interest to PPS Members

As noted in the previous issue of the PPS Newsletter, papers of general interest will appear in the Newsletter for the benefit of PPS members. In this issue a paper is presented on Molecular Modeling by Prof. Doros Theodorou, the 2006 Danckwerts Lecture award winner (AIChE, IChemE, etc.), from the National Technical University of Athens (NTUA) in Greece. More about Prof. Theodorou's research interests can be found in the web page:
http://comse.chemeng.ntua.gr/

Can molecular modeling predict polymer properties relevant to processing?

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How will the viscosity and moduli of a polymer melt change if one introduces a chemical modification in the structure of the repeat units? How can one tailor the composition and microphase-separated morphology of a block copolymer-based adhesive to achieve best performance? How can one control the permeation of gases through a membrane or packaging material by appropriate design of the chemical constitution of chains? Questions such as these have traditionally been addressed through experimentation or phenomenological correlations. Nowadays, however, advances in molecular simulation methods and the availability of increasingly powerful computers have brought these questions within reach of rigorous, predictive, statistical mechanics-based molecular modeling.

A formidable challenge in trying to predict polymer properties computationally lies in the very broad spectra of characteristic times for motion in macromolecular systems. These range from the periods of bond vibrations (10^{-14} seconds) to the longest relaxation times of polymer melts (10^{-3} to 100 seconds for typical molecular weights) to the time scales for volume and enthalpy relaxation (physical ageing) of glassy systems (exceeding years, or 10^{7} seconds). By comparison, the longest time that can be accessed by an atomistic molecular dynamics simulation (numerical solution of Newton's equations of motion for all particles in a material) is on the order of 10^{-6} seconds. Within the last decade, it has become apparent among computational polymer scientists and engineers that progress can be achieved only through the development of *hierarchical* modelling approaches consisting of many levels, each level addressing phenomena over a specific window of time and length scales, receiving input from more fundamental levels and providing input to more coarse-grained ones. Such a hierarchy [1] may include quantum chemical calculations to extract potential energy functions from chemical constitution; atomistic energy minimization, Monte Carlo, molecular dynamics, and transition-state theory computations; mesoscopic kinetic Monte Carlo, self-consistent field theory, dynamic density functional theory, Brownian dynamics, or dissipative particle dynamics simulations; and macroscopic finite element-based computations based on the continuum engineering sciences. Creative design and application of multiscale methodologies can bridge the gap between chemical constitution and macroscopic properties.

At the atomistic simulation level, powerful connectivity-altering Monte Carlo methods can now fully equilibrate long-chain melts [2], yielding excellent predictions for density, packing, and chain conformational characteristics in the bulk and at interfaces. Segmental friction coefficients and their temperature dependence can be extracted from molecular dynamics simulations [3]. Through topological analysis, long-chain melt configurations can be reduced to entanglement networks [4] appropriate as starting

points for mesoscopic slip-link simulations of melt relaxation and flow. Recent applications have shown that such hierarchical schemes can predict reliably the effect of changes in monomer chemical constitution and chain architecture (e.g., introduction of short-chain branching) on rheological properties.

Coarse graining, i.e., the systematic reduction of an atomistic polymer model into one involving fewer degrees of freedom, is an effective way to reduce computational cost in polymer simulations ([3], Figure 1). Coarse-grained representations are useful in the context of self-consistent field theories, which can provide valuable predictions for the expected morphology of multicomponent self-organizing systems containing block copolymers and for elucidating structure at polymer surfaces, polymer/polymer and polymer/solid interfaces [5], and in nanocomposites.

Sorption equilibria and diffusivities of gases and solvents in rubbery polymers can be predicted thanks to recent advances in Monte Carlo and molecular dynamics methods. For glassy polymers, where diffusivities are too low to be captured by molecular dynamics, methods based on transition state theory come to the rescue. The diffusive progress of a penetrant molecule through the polymer matrix can be envisioned as resulting from a succession of infrequent jumps between clusters of accessible volume, whose paths and rates are computable by geometric and energetic analysis [6].

A major advantage of molecular modeling is that it can predict a wide variety of properties starting from the same fundamental input concerning the building blocks (molecules, atoms, ions) of a material. It can also bring out the mechanisms, i.e., why does a polymeric material exhibit the properties that it does and how are these properties expected to change if we change something in the chemical constitution of the material? Complementary experimental work is always valuable for validating methods at all levels of the modeling hierarchy and for realizing design principles reached by the modeling.

Molecular modeling of polymers is far from routine work. It needs inspiration and dedication. It is truly fascinating to enlist one's basic scientific knowledge and mathematical skills in order to understand and predict why polymeric materials behave the way that they do and how their performance could be improved for specific applications.

References

[1] Kotelyanskii, M.J. and Theodorou, D.N., Eds. *Simulation Methods for Polymers*, Marcel Dekker: New York , 2004.

[2] Theodorou, D.N., in: Nielaba, P., Mareschal, M. & Ciccotti, G. (Eds.), *Bridging time scales: Molecular simulations for the next decade*. Springer-Verlag: Berlin, 2002, pp. 69-128.

[3] Theodorou, D.N. *Chem. Eng. Sci.* **62**, 5697-5714 (2007).

[4] Tzoumanekas, C., Theodorou, D.N., *Current Opinion in Solid State and Materials Science* **10**, 61-72 (2006).

[5] Theodorou, D.N. , in *Computer Simulations of Surfaces and Interfaces*; Dünweg, B.; Landau, D.P.; Milchev, A., Eds.; Kluwer Academic Publishers (NATO Science Series II/114): Dordrecht, 2003, pp 329-419.

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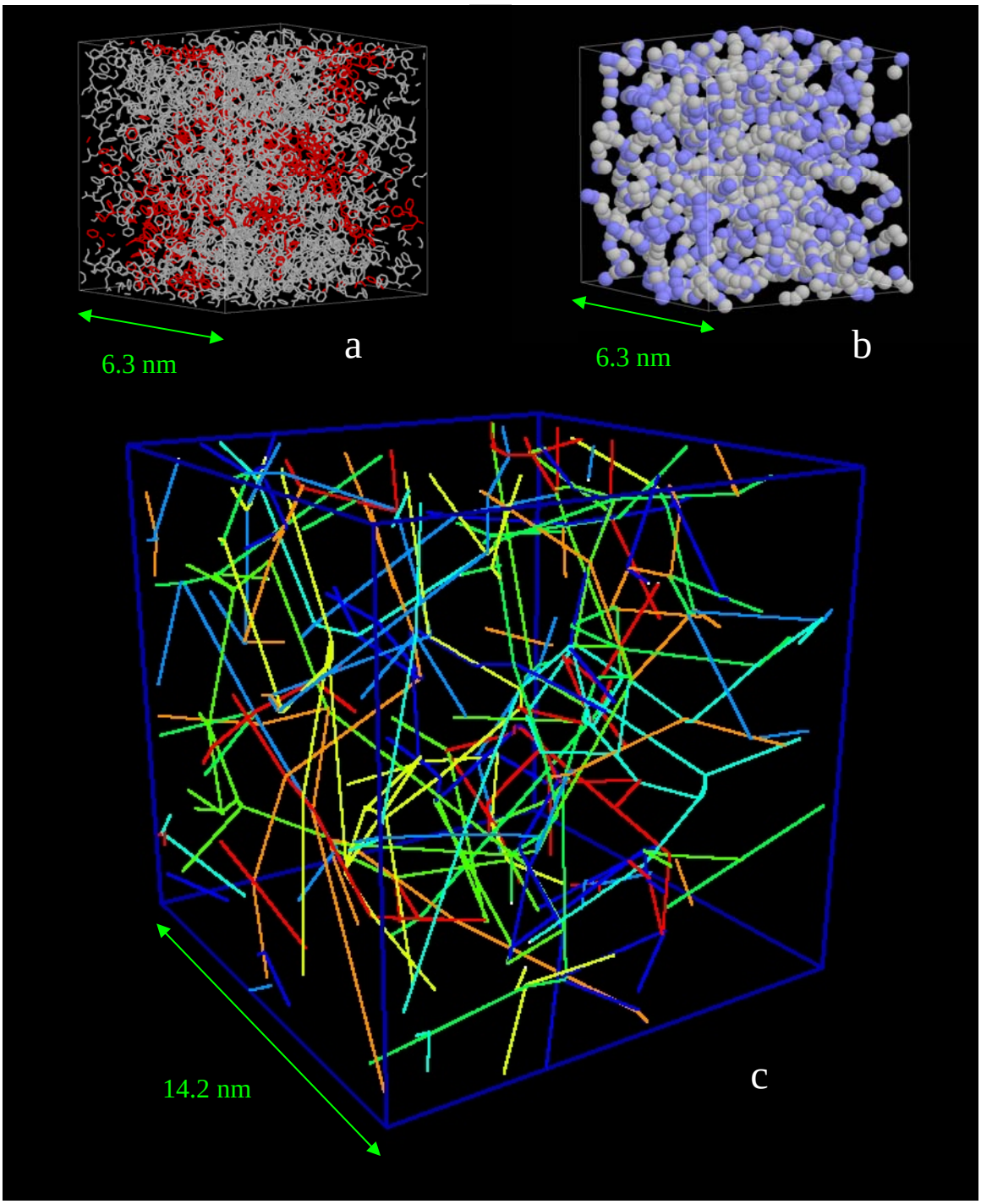

Figure 1: Three levels of representation of atactic polystyrene melt specimens at 500K and 1 bar: (a) detailed united-atom model; (b) Coarse-grained model, wherein each dyad of monomers is represented as an interaction site (superatom); (c) entanglement network; different reduced chains (primitive paths) are represented in different colors.