

Division IV: Polymer Division

The objective of this report is to summarize the activities of Division IV from the Bureau Meeting of 11-13 April, 2014 in Coimbra (Portugal) until the Bureau Meeting of August 2014 in Busan (Korea) and to discuss future goals for the Division.

In June 2015, Polymer Division has completed the following roster for the 2016-2017 biennium:

President: G. Russell; Vice-President: Christine Luscombe; Secretary: M. Walter; Past President: M. Buback;

Titular Members: Sabine Beuermann (Polymerization Kinetics and Processes); J. He (Structure and Properties of Commercial Polymers); I. Lacik (Conferences); M. Sawamoto (Strategy); Natalie Stingelin (Terminology); Y. Yagci (Trends in Polymer Science);

Associate Members: R. Advincula (Education); D. Auhl (Structure and Properties of Commercial Polymers); M. Hess (Education); R. Hiorns (Terminology); R. Hutchinson (Polymerization Kinetics and Processes); G. Moad (Terminology);

National Representatives: R. Adhikari (Nepal); C.-H. Chan (Malaysia); Voravee P. Hoven (Thailand); C.-S. Hsu (China/Taipei); R. Jones (UK); D.-S. Lee (Korea); M. Malinconico (Italy); Olga E. Philippova (Russia); C. dos Santos (Brazil); J. Vohlidal (Czech Republic);

Interdivisional Activities

The Polymer Division is involved in several interdivisional projects, in particular with Division VIII. Division IV remains a committed member of the Interdivisional Subcommittee on Materials Chemistry. Contacts continue to exist with the Committee on Chemistry and Industry (COCI).

Polymer Division Meeting

The Polymer Division Meeting was held in Chiang Mai (Thailand) on July 4-5, 2014 with 34 attendees. A list of the current projects is compiled by the Secretariat and is available at the IUPAC website. Division IV is very active in carrying out IUPAC projects. The Chairperson of each Subcommittee monitors the projects including progress reports from the Task Group Leaders. As the reports on the projects are contained in the Minutes of the Division Meetings posted on the IUPAC website, only brief comments about the individual Subcommittees will be presented here. The activities of IUPAC Polymer Division are primarily carried out within the following four Subcommittees.

Subcommittee on Polymer Terminology (SPT)

The 2014 meeting of the Subcommittee was held at Chiang Mai (Thailand) between June 29 and July 3, 2014 prior to the IUPAC World Polymer Congress. Twenty-nine members and observers were attending. Via Skype four more members were

participating. SPT has had a very productive year, with projects being developed through electronic communication. Nevertheless the annual face-to-face meetings are extremely important for discussing the milestones and for resolving critical issues. It should be noted that six new members have joined SPT over the last three years.

After completion of several initiatives, five new projects have been launched, mostly in cross-science areas, e.g., where polymers are of interest to energy, health and medicine as well as to computer modelling. The completion of the project "Nomenclature for chemically modified polymers" should be particularly mentioned, as this is seen as the flagship document for the extension of modern polymer nomenclature.

In the period covered by this report, the Subcommittee has worked on 18 projects, of which five have been concluded successfully, and one is close to being finished. As planned in Chiang Mai, five project applications have been submitted, with three still under review, and two of them already approved and funded.

The recent outcome of SPT work has been published in *Pure Appl. Chem.* 86 (2014) 1003–1015, *Pure Appl. Chem.* 87 (2015) 71–120; *Pure Appl. Chem.* 87 (2015) 307–319, as well as in numerous Wikipedia pages now carrying IUPAC definitions through the project 2011-013-2-400 "Updating Wikipedia: Synchronizing Polymer Definitions and Terminology" and through internet entries for the Multilingual Polymer Glossary which is produced within the project 2007-008-1-400 "Development of a Multilingual Encyclopedia of Polymer Terminology". Moreover, the Purple Book was made freely available on the IUPAC website.

The following projects have been successfully reviewed and most likely will be funded shortly:

- 2014-034-2-400 "Nomenclature for polymeric carriers bearing chemical entities with specific activities and names";
- 2014-033-1-400 "Nomenclature and terminology relevant to lactic acid-based polymers: synthesis, structure, properties, applications and degradation";
- 2015-012-1 "Terminology of Tissue Engineering and Regenerative Medicine in Polymer Science";
- 2015-013-1-400 "Brief Guide to Polymerization Terminology";
- 2015-014-1-400 "Guide (and Brief Guide) to Polymer Semiconductors".

The project on "Source-based nomenclature of single-strand organic polymers and copolymers will be sent to public review shortly.

The following projects are currently addressed, but have end-dates after August 2015: "Terminology and structure-based nomenclature of dendritic and hyperbranched polymers", "Terminology on separation of macromolecules", "Terminology for conducting, electro-active and field-responsive polymers", "Preferred names for polymers", "Revision of the web-based guide: IUPAC Recommendations on Macromolecular Nomenclature – Guide for Authors of Papers and Reports in Polymer Science and Technology", "Definitions and notations relating to stereochemical aspects in polymer science", "Terminology for chain polymerization", "Keywords in polymer science journals", "Terminology and nomenclature of inorganic and coordination polymers (TINCOPS) – an extended revision of Nomenclature for regular single-strand and quasi-single-strand inorganic and coordination polymers",

“Terminology of nanomaterials and nanotechnology in polymer science” and “Structure-based nomenclature for regular linear star, comb and brush polymers”.

There is an extended list of projects in preparation for submission, e.g., “Definition of terms relating to the ultimate mechanical properties of polymers”; “Brief Guide to the Characterization of Polymers”, “Brief Guide to Polymer Microstructure”; “Polymers from renewable and recycled sources”; “Terminology for constitutionally-dynamic polymers”, “Polysiloxanes”; “Polymer Inorganic hybrids”, “Polymers for 3D printing”; “Evaluation of polymer crystals”.

Special interest focuses on the project: “Updating Wikipedia: Synchronizing Polymer Definitions and Terminology” which aims at eliminating, for the area of polymer science, discrepancies between Wikipedia and IUPAC definitions. Beyond the interest in improving the polymer-related quality of Wikipedia entries, the entire set of IUPAC definitions and associated PAC publications should be linked, by an appropriate window, to Wikipedia. According to Wikipedia practice, some additional text, explanations and perhaps some historical background will be provided to meet the expectations of the wide readership. Polymer-relevant Wikipedia entries have to be checked against existing Division IV Terminology & Nomenclature documents and links have to be established. New IUPAC documents will be checked by the task group for linking with Wikipedia. Questions concerning graphics and videos also need to be addressed. Special measures need to be taken to identify later changes of the open encyclopedia and to find ways for recovery of the original text of the “IUPAC window”

Subcommittee on Structure and Properties of Commercial Polymers

This Subcommittee meets at least once per year to identify and work on scientific projects, mostly of an experimental nature. From seven scientists in 1963, the membership has increased to 68 from 12 countries. Twenty-seven scientists are from industry and 41 from academia or from research institutions. The SC thus continues to have a well-balanced membership. The SC projects are initiated by industry and funded by the participant organizations with an additional IUPAC budget for travelling costs. To maintain membership in the Subcommittee it is mandatory to participate in at least one project and to attend at least one meeting every two years. The 2015 Subcommittee meeting, which was No. 73, was held in Prague (Czech Republic), April 22-24, 2015, with 24 participants from 8 countries. The East Asian meeting of the SC was held in Luoyang, China, November 19-20, 2014, with 20 participants from three countries. The next meetings will be held November 4-5, 2015 in Busan (Korea) and April 2016 in Europe.

Two papers have recently been published with the serial numbers referring to the total output of papers over the years: [91] K. Wang, F. Wu, W. Zhai, W. Zheng, “Effect of polytetrafluoroethylene on the foaming behaviors of linear polypropylene in continuous extrusion”, *J. Appl. Polym. Sci.* 129 (2013) 4 and [92] M. Laun, D. Auhl, R. Brummer, D. Dijkstra, C. Gabriel, M. A. Mangnus, M. Rüllmann, W. Zoetelief, U. Handge, “Guidelines for checking performance and verifying accuracy of rotational rheometers: viscosity measurements in steady and oscillatory shear”, *Pure Appl. Chem.* 86 (2014) 1945–1968.

The projects 2010-029-3-400 “Relation between rheological properties and foam processability for polypropylene” and 2005-023-2-400 “Microstructural, melt processing and mechanical properties of compatibilized PA6/ABS Blends” have been completed. The current SC projects are on: “Guidelines for shear rheometer calibration and performance check” with a first paper in *Pure Appl. Chem.* 86 (2014) 1945–1968 and “Elongational rheometry devices for shear rheometers” and “Characterization, rheology and mechanical properties of high and ultra-high molecular weight polyethylene”. Four draft versions will serve the purpose of finalizing the projects on molar-mass analysis, on DSC characterization, crystallinity and crystallization, on micro-mechanics, entanglement and grain boundaries, and on macro-mechanics, cracks and wear behavior.

Feasibility studies are in preparation on the “Comparison between experiment and simulation of extrudate swell”; “Rheological behavior of thermoplastic polyurethane”; “Characterization of molecular structure”; “Transparent propylene/butane-1 random copolymer”; “Anti-bacterial and anti-mildew PP resin”; and “Deformation behavior of neck-forming polymers”.

Subcommittee on Polymer Education

The Subcommittee has been successfully chaired by Werner Mormann over many years. He will finish his service by the end of 2015. Chris Ober agreed to take over as an interim chair. The activities of SPE are directed towards supporting courses, workshops, and conferences, with particular emphasis on service for the developing world and for younger scientists.

As a recurrent event, the 18th UNESCO/IUPAC Postgraduate Course in Polymer Science will take place in Prague under the leadership of Pavel Kratochvil. University graduates and PhDs from countries with limited research facilities are given the opportunity to acquire knowledge about recent advances in polymer science to be used for the promotion of polymer science in their home countries. So far, the courses have been attended by 138 graduates from 20 countries with an output of 285 publications in international journals and 329 communications at international meetings associated with more than 4500 citations.

As another recurrent event, the IUPAC-endorsed POLYCHAR 23 Conference (World Forum on Advanced Materials) has been held in Lincoln (Nebraska), May 11-14, 2015. This conference enjoyed an IUPAC grant for support of students from developing countries. The 13th Annual UNESCO/IUPAC Workshop and Conference on Macromolecules & Materials will be held September 7-10, 2015 at Port Elizabeth (South Africa).

A two-days symposium on Polymer Education has been organized by the Subcommittee during Macro 2014 at Chiang Mai. The situation of polymer education in South-East Asia has been specifically addressed. Extended manuscripts will be included into volume 355 of the *Macromol. Symp. Series* (September 2015). The SC project on “Enhancing Educational Website for Polymer Chemistry” has been approved. Under the leadership of Chris Ober, this initiative will also investigate the

traffic that comes to the website and will provide information about matters of prime public interest.

As a finalization of the IUPAC transnational/transcontinental call on Polymer Science, organized and carried out under the auspices of the Subcommittee on Polymer Education, a symposium has been arranged during MACRO 2014 at Chiang Mai with presentations by the successful teams of the first round.

Subcommittee on Modeling of Polymerization Kinetics and Processes

This Subcommittee, which is co-chaired by Sabine Beuermann (Clausthal, Germany) and Robin Hutchinson (Kingston, Canada), has 45 members from 15 countries. The Subcommittee is active in critically evaluating kinetic parameters of polymerization processes and establishing reliable methodologies.

Two meetings of the Subcommittee were held, during MACRO 2014 at Chiang Mai in July 2014 and during the ACS National Meeting in San Francisco, August 2014. Within the kinetic activities of the Subcommittee, a paper on the propagation rate coefficient of methyl acrylate has been published (*Polym. Chem.* 204 (2014) 5). This recent paper has already been cited 10 times. The continued major interest in this kinetic work of the Subcommittee is demonstrated by the enormous and continuously increasing number of citations, with the benchmark paper on styrene being cited more than 500 times so far. It is pleasing to note that the reference data released by this IUPAC Subcommittee are accepted as benchmark values worldwide.

Monomer	Journal	Year	Web of Science Citations (July 1, 2015)
1. Styrene	<i>Macromol. Chem. Phys.</i>	1995	540
2. Methyl Methacrylate	<i>Macromol. Chem. Phys.</i>	1997	415
3. Alkyl Methacrylates	<i>Macromol. Chem. Phys.</i>	2000	175
4. <i>n</i> -Butyl Acrylate	<i>Macromol. Chem. Phys.</i>	2004	213
5. RAFT mechanism	<i>J.Polym. Sci. A</i>	2006	293

Related to the kinetic work, studies into the accurate molar-mass analysis of polymers have been carried out by the Subcommittee, resulting in the paper: “SEC Analysis of Poly(Acrylic Acid) and Poly(Methacrylic Acid), *Macromol. Chem. Phys.* 216 (2015) 23-27. Within a separate Subcommittee project, the kinetics of initiator decomposition is investigated, chiefly by Graeme Moad. A comprehensive manuscript, which provides a critical overview of the kinetics and mechanisms of commercially available dialkyldiazene initiators is in the process of being published in *Prog. Polym. Sci.*.

Current Subcommittee projects deal with “Chain-length dependent termination kinetics”; “Vinyl acetate propagation kinetics”, and “Rate coefficients for styrene radical polymerization”. In preparation is a project to be chaired by Atsushi Kajiwar

on the EPR spectra of relevant radicals occurring in conventional and in reversible-deactivation polymerizations.

The project “Mechanistic details of RAFT polymerization”, which has induced a remarkable flurry of publication activity, has essentially been finalized by the comprehensive manuscript on dithiobenzoate-mediated RAFT polymerization prepared by task-group member Graeme Moad in *Macromol. Chem. Phys.* **215** (2014) 9-26.

The next meeting of the Kinetics and Mechanism Subcommittee will take place during Pacificchem 2015.

Polymer Division Conferences

IUPAC-endorsed polymer-related conferences attract participants from all around the world. Endorsement is judged on the criteria of scientific quality, significance and suitability of the conference, evidence of sufficient advanced planning, suitable time spacing of conferences of a similar type, rotation of leadership for conferences in a series and a geographically diverse International Advisory Board, participation of industrial chemists and women as speakers and as members of the International Advisory Board.

The IUPAC-endorsed polymer symposia and conferences are listed on the IUPAC website. Ten such conferences are held in 2015 under the auspices of Polymer Division. So far, the following conference proceedings have been published in “Macromolecular Symposia”: *Macromolecules and Materials* (Vol. 337); *Polymer Spectroscopy* (Vol. 339); *Molecular Order and Mobility in Polymer Systems* (Vol. 348); *Ionic Polymerization Part I* (Vol. 349) and *Ionic Polymerization Part II* (Vol. 350).

World Polymer Congresses

The WPCs are the flagship conferences of Polymer Division held in the even years. Actually, these MACROs are the largest polymer congresses worldwide. MACRO 2014 took place at Chiang Mai (Thailand) from July 6-11, 2014. Turkey will organize MACRO 2016 in Istanbul and Australia has received preliminary approval for MACRO 2018 to be held in Cairns. The largest IUPAC Polymer Division-endorsed conference of this odd year was the European Polymer Federation Congress in Dresden, June 21-26, 2015 with more than one thousand attendees and with an opening address being given by the President of IUPAC Polymer Division..

Further points of note from discussion at the Polymer Division Committee Meeting

The importance of early recruitment of new members for the division was discussed, as was the duration of projects. The project lifetime should be carefully estimated on the basis of the specific work program and should be checked by the subcommittee chairs.

The Polymer Division enormously benefits from the awards that are generously financed by companies and are presented during the biennial WPCs, i.e., the DSM–IUPAC Material Science Award, the Samsung–IUPAC Young Polymer Scientist Award, and the Polymer International–IUPAC Award. It has been discussed whether an ‘Award Coordinator’ should be installed to take care of this important initiative, prepare the calls and make sure that worldwide attention is paid to these awards and that the best candidates will be identified. The prestigious DSM–IUPAC prize (50.000 Euro) has been awarded at MACRO 2014 for the fourth time.

The following initiatives continue to command attention from the Polymer Division: involving younger scientists and colleagues from industry; strengthening polymer activities in developing countries; improving the role of the Polymer Division in education; strengthening the IUPAC label and enticing organizations to ask for IUPAC advice; broadening IUPAC service in the areas of terminology and nomenclature and in providing reliable benchmark data of polymerization-related rate data; recommending reliable techniques for measurement of polymer-relevant parameters and coefficients; strengthening the role of NRs by asking them to act as ambassadors for both sides, viz. their IUPAC Division and their NAO; recruiting excellent candidates for service to IUPAC.

Michael Buback
Division IV President
July 3, 2015