

# IUPAC and Commercial Polymers

## IUPAC Working Party on Structure and Properties of Commercial Polymers—History, Output, and Future Prospects

by D.R. Moore and H.M. Laun

It is nearly an axiom that working groups within organizations of almost all sorts come and go with need, interest, and fashion. Thus, the continuous existence of a Working Party (WP) within IUPAC for over 40 years is, to say the least, unusual. Nevertheless, since 1963 academic and industrial scientists with similar interests have contributed to the distinguished history of the Working Party on Structure and Properties of Commercial Polymers. Today the WP functions as a formal Subcommittee of the Macromolecular Division.

The WP has a robust current membership of 66 scientists from 17 countries, representing industry, universities, and institutions. It has held 70 meetings and published more than 80 scientific papers in its 40 years; it is largely self-governing and elects its own executive officers.

As so often is the case, its beginnings were humble. At the first meeting of the WP in 1963 there were only 7 scientists in attendance. However, the numbers of participating scientists, companies, and institutions grew quickly. The first publication, *The Relationship of Performance Characteristics to Basic Parameters of Polymers. I: A Collaborative Study of Polystyrene Using Torsion Pendulum and Impact Methods*, was published in 1968. Six laboratories contributed to this publication: BASF, DOW, Monsanto, Solvay, TNO, and Technická Prague.

The first publication on the collaborative study of polystyrene and polyethylene melts was published by J. L. S. Wales in 1969. Contributing laboratories were Monsanto, Péchiney-Saint-Gobain, Solvay, and TNO. Polyvinyl chloride (PVC) was an early focus, especially its mechanical and capillary-flow properties. Initially most participating scientists were from U.S. and European plastics industries, but they were increasingly supplemented by scientists from academia worldwide, including the then Soviet Union. In addition to the early work on polyolefins, PVC, and polystyrene, there were also excursions into polypropylene film.

In its first 10 years, the WP was particularly concerned with how to relate mechanical and rheological

measurements to the practical world of plastics processing and performance. In one project, the rheological properties of three low-density polyethylene samples were related to their tubular-film-blowing characteristics. From this work, the importance of extensional-flow testing became obvious and motivated further efforts in the development of extensional rheometers.

In the period between 1963 and 1980, the WP held 37 meetings, all of them in Western Europe. However, there was a strong presence from the USA in the membership of the group and the WP finally held its first meeting in the USA in 1981. In addition, two regional subgroups were established in the early 1980s, one in Japan with members from Japan, China, and Korea, and another in eastern Europe, with members from Czechoslovakia, Hungary, Poland, and the USSR. The motivation for the formation of these subgroups was to expand membership on a global basis and to ease travel restricted by cost or political conditions. These subgroups established their own projects and reported to the main WP.

The early 1980s was a time of expansion for the WP. There were projects on the impact behavior of injection moldings led by C. B. Bucknall, and feasibility studies for understanding polymer blends in terms of processing-structure-property relationships. In particular, in projects led by H. M. Laun and P. Hope, the WP looked at suitably selected model systems for miscible and immiscible blends based on technical polymers. In East Asia there were also projects relating to structure-property relationships for polybutadiene-rubber blends.

A significant development involved establishing projects on contemporary polymeric materials and systems. Polymeric fiber-reinforced composites were fast emerging and the WP was well placed to contribute to this area. Studies were started by D. R. Moore and J. C. Seferis on continuous carbon-fiber reinforced semi-crystalline polymers, followed by projects led by A. Cervenka and P. S. Allan on discontinuous fiber-reinforced polymeric systems.

The traditional interest that the WP has had in linking rheological properties to processing continued. In two projects, J. L. White explored a link between rheological properties and unstable melt-spinning for linear and branched poly(ethylene terephthalates), and examined the stability of extrusion, melt spinning and tubular film extrusion for some high-density, low-density, and linear-low-density polyethylene samples.

The final decade of the 20th century was a time of considerable achievement; it was also what can be

described as a political period. IUPAC was undergoing considerable restructuring; this naturally had a profound influence on the organizational aspects of the WP, though almost none on its activities.

The emergence of *détente* and political freedom within continental Europe provided new ease of access and communication between scientists in the East and West. The WP held meetings in Czechoslovakia (just before it became the Czech and Slovakia Republics) and in Poland in 1992 and 1993, respectively. The WP closed the East-Europe subgroup after these meetings and integrated the scientists involved into the main group.

The integration of the East Asian subgroup was more difficult because there were more substantial cost barriers to meetings at a single location. An arrangement was established whereby the members of the subgroup became members of the WP, but could hold a research meeting in their area once a year. This was consolidated with a full meeting of the WP in Korea in 1996. Ten of the 28 participants were members from Europe, USA, and Canada.

Polymeric fiber-reinforced composites became of significant interest in the 1990s; in particular, composites with a potential for use in primary aerospace structures. A project led by D.R. Moore and J.C. Seferis studied two materials systems of continuous carbon-fiber reinforced thermoplastics. A key feature in the overall study was to find a way of accommodating the massive anisotropy in these fiber-reinforced composites whilst retaining an ability to measure some conventional but important properties.

A second fiber-reinforced composites study was led by P. S. Allan and A. Cervenka and became the largest single project undertaken by the WP, with 21 participating laboratories and 7 published papers. The project was concerned with the processing and properties of injection-molded discontinuous fiber-reinforced thermoplastic composites, with the aim of providing characterization of

the processing-property-structure relationships that characterize this complexity.

A third composites project led by D. R. Moore and A. Cervenka focused on future requirements for the characterization of continuous-fiber-reinforced composites. In this study, contributing scientists reviewed some of the history of processing and properties of these composite materials and tried to identify factors that would be important in the future. This was the first WP project with a philosophical rather than an experimental output.

Meanwhile a major strategic thrust was being developed on immiscible and miscible blends. The first blends project, coordinated by A. P. Plochocki, was a joint study of the effect of mixing and processing conditions on the phase morphology and rheology of polystyrene/low-density polyethylene (PS/LDPE) blends. A second study, led by P.S. Hope and J.E. Curry, focused on the reactive blending of immiscible blend components.

A project on miscible blends was co-ordinated by H. M. Laun, J. Lyngaae-Jorgensen, and V. Alstädt. It focused on the preparation of blends of various morphologies, but with the same composition of the constituents and the study of the effects of morphology



*Participants at the Working Party IV.2.1 research meeting in Ludwigshafen (2003), hosted by H.M. Laun at BASF. Front row from left: S. Monsheimer (Degussa), U. Handge (ETH Zürich), H. M. Laun (BASF), A. Machado (Guimares), Ch. Chai (BP chemicals), W. Gleissle (Karlsruhe), G. Ourieva (Exxon Mobile), J. Lyngaae-Jørgenson (Lyngby). Middle rows: P. Pelz (Freudenberg), M. Rüllmann (BASF), D. Stocks (ICI), R. S. Bailey (ICI), D. Dijkstra (Bayer), J. Meissner (ETH Zürich), R. Koopmans (DOW), V. Rouyer (BP Solvay), T. Inoue (Kyoto), G. Biebaut (Shell), H. Steininger (BASF), V. Alstädt (Bayreuth). Back rows: R. Brummer (Beiersdorf), F. Ramsteiner (BASF), W. Zoetelief (DSM), B. Hochstein (Karlsruhe), I. Fortelny (Prague), C. Gabriel (Basell), U. Göschel (Stuttgart), E. Piorkowska-Galeska (Lodz), C.B. Bucknall (Cranfield), T. Tagigawa (Kyoto), K. Nitta (JAIST), A. Galeski (Lodz), F. Langouche (Solvay), E. Wassner (Elastogran), B. Ouriev (Bühler AG).*

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on rheological and mechanical properties. The constituents were very similar in their viscoelastic behavior. The shift of the regime of miscibility by simple shear flow was investigated, and the observed morphology changes in oscillatory shear were compared with available theories for droplet/matrix and cocontinuous structures. The composition and temperature dependence of the interaction parameter  $\chi$  was quantified by means of neutron diffraction and cloud-point studies for blends of P $\alpha$ MSAN with PMMA and with poly(methylacrylate-co-methylmethacrylate). Finally, the effects of morphology on the mechanical properties of the blends were investigated.

C. B. Bucknall and M. Kozłowski undertook another large project on blends. In this work, the addition of "core-shell" rubber particles to thermoplastic matrix materials was studied for enhancement of toughness with an aim of understanding the mechanisms involved in the toughening process. Two rubber-particle systems were selected having quite different glass-rubber transition temperatures. These were blended with four different thermoplastic matrix materials at the same volume concentration of the rubber. Mechanical and rheological properties of these systems were investigated, and structural and deformational mechanisms were discussed for tensile impact behavior, dart-drop and notched bending test, and fatigue behavior. A transmission-electron-microscopic investigation of *in situ* deformation was published.

Following the IUPAC Strategy Development and Implementation Committee recommendations of 1998, the Macromolecular Division moved to a project-driven system. As a direct consequence, starting in 2000 the WP no longer held official status within IUPAC and became an ad-hoc working group. In the reorganized division, the chairman of the WP became one of the characterization coordinators within the division, while both the secretary of the WP and the chairman of the East Asian Research Meeting acted as task group chairmen of projects.

R. B. Bailey (Secretary) became task group chairman of a five-year project on "Quantifying scratch resistance of commercial polymers." The goal is to consider the range of scratching, abrasion, and erosion techniques used in the plastics industry and to apply a more fundamental understanding of the issues that contribute towards scratch resistance. In stage 1 of the project, key links between bulk and coating mechanical properties and scratch and abrasion resistance are to be identified using generic techniques to manufacture materials with a "scratch-

resistant" surface on acrylic and polycarbonate polymers. Stage 2 will focus on emerging and novel scratch-resistant coatings.

S. C. Kim became task group chairman of a three-year project on "Structure and properties of cyclic olefin copolymers (COC)." Here, the focus is on relating the chemical structure of commercially available COCs to rheological and processing properties as well as to optical and mechanical properties in the solid state.

In 2002, a former feasibility study of the East Asia members became a three-year project on "Structure and properties of polyester elastomers composed of poly(butylene terephthalate) and poly( $\epsilon$ -caprolactone)," with T. Tagigawa as task group chairman. Subtopics of the joint study are molecular structure, rheological properties, rubber elasticity, aggregate structure and deformation mechanism, and blends with other polymers.

The WP amended its rules to require that all communications be conducted via e-mail. A WP homepage <[www.launweb.de/iupac](http://www.launweb.de/iupac)> was set up to keep the documentation on projects, reports, people, and actions continuously updated. It contains a public sector open to anyone and a private sector for members only.

Under new IUPAC guidelines, projects are to last about three years. Based on WP experience, this is often not enough time for voluntary and unfunded joint experimental work. Therefore, proposals for new projects within the WP are converted into feasibility studies in which the outline and goal of the work, the suppliers of the material, and contributors and coordinators are defined. Only then is the project application submitted to IUPAC via the Macromolecular Division.

In 2003, the WP again became an official part of the IUPAC Macromolecular Division and was recognized as the Subcommittee on Structure and Properties of Commercial Polymers, a most welcome change of status for the 40th anniversary of the group. Studies that will occupy the group over the next few years include the following:

- structure and properties of linear and crosslinked, structural PVC foams
- flow properties of ceramic and metal injection-molding feed stocks
- recommendations for data presentation applicable to mechanical and rheological measurements of polymers
- critical check of capillary-flow predictions using viscoelastic finite-element simulation and low-density polyethylene literature data
- the role of stress-induced cavitation in mechanical



- performance of semi-crystalline polymers
- rheological characterization of polyamides
  - future developments of new materials based on commodity polymers by physical structure and morphology alteration
  - investigation of morphology parameters governing the properties of melt-processable filled polymers

The direction of the WP was set in its early days. It was broad ranging and flexible, and it has not changed significantly over the years. The group existed within the IUPAC organizational structure, which monitored but did not define its activities. The group's project base was self-defined and the consequences of this are extremely important.

First, the WP has consistently initiated projects that it knew were of relevance to industry, academia, and the world at large. Also, in a general sense, the work had to be convincing to the paymasters, namely, industrial managers or academic supervisors. It was, therefore, crucial that the appropriate skills be present and active in the WP.

Second, the members of the WP find great value in working with like-minded scientists on a global basis; it offers contacts and networks that would be difficult to establish by any other means. In addition, there is considerable value in scientific projects in which an individual (or his or her organization) is funding only a fraction of the cost.

Third, the definition of a project by its task group members ensures that the project is of contemporary value and importance. Common themes that are important to several industrial scientists can be turned into a useful, but non-competitive project. Further, seeking academic involvement often provides useful input from leading experts. Despite moves within the broader IUPAC organization to generate and define projects on a top-down basis, it will be vital to retain some projects that come from the bottom-up approach of the WP.

The driving force behind the WP has always been the motivation to obtain value (to them and their businesses) from participation in the group. If value is obtained, participation is funded. This principle has guided the WP for 40 years through changing economic climates; there is no reason to assume it won't work for another 40 years.

The international network of scientists making up the WP will continue to pursue projects that have contemporary value and that lead to publications. The types of materials and the approaches used will no

doubt change, but there will always remain issues relating to polymeric systems or particular properties that will need to be characterized and understood.

There is likely to be demand for shorter projects in the future, as impatience for returns on investment is always present. In a recent trial of a possible approach, a philosophical document on the future requirements for the characterization of composites was written. This type of approach is based solely on an existing knowledge base, eliminating the need for conducting new measurements. The decline in major corporate organizations in the chemical industry suggests that the need for such an approach could be larger than we might predict.

Some completed projects have provided comprehensive data on commercial polymers that are still available and may be used for further research outside of the WP. Recent examples are poly( $\alpha$ -methylstyrene-co-acrylonitrile) (P $\alpha$ MSAN) and poly(ethyl methacrylate) (PMMA) and their blends. Besides a rheological and mechanical characterization of the constituents and their blends, there is valuable information available on the interfacial tension as well as the interaction parameter  $\chi$  as a function of temperature and composition. Further studies on this system are specifically encouraged.

There are also educational values that the WP could satisfy. A new recruit could serve a few years on the WP in order to become acquainted with the network of activities and people or merely to learn a different approach to conducting research or a project.

It is obvious that the future lies with the people involved and their commitment to the broader aims of the WP. It will depend on whether they involve others in the activities of the group because they see and appreciate its benefits. Finally, it will depend on whether they communicate the values and virtues of the WP and ensure that their organizations support their continued involvement.

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D. Royston Moore <r.moore@imperial.ac.uk> has been involved with the WP for more than 10 years and is now an IUPAC Fellow; he is now at the Mechanical Engineering Department of the Imperial College in London, U.K.; H. Martin Laun <martin.laun@basf-ag.de> works at the Polymer Research Division of BASF Aktiengesellschaft in Ludwigshafen/Rhein, Germany.