

Macromolecular Division:

Report of Activities August 1997 - August 1999

Most Division activities occur through its three Commissions. In addition, a major initiative has been to work out means of implementing the SDIC recommendations. This has occupied considerable time for MMD this biennium, including a series of 4 meetings on this at the MMD meeting in July 1998 in Australia plus extensive electronic discussion.

- The main activity of the Division as such was through the World Polymer Congress (Macro98) held July 11-15 1998 at the Gold Coast, Australia, which attracted 1200 registrations from 41 countries.
- The MMD also provided support for the Prague Postgraduate Course in Polymer Science, under joint auspices of UNESCO and IUPAC. Most of the attendees are citizens of the former Soviet block countries, where the research facilities are now very modest.
- The Division is supporting a project on "Education in Polymer Science in the Universities of the World", under Prof Khokhlov, based at Moscow State University. All curricula of the polymer science educational programs, description of lecture courses and practical exercises for the universities in Russia have been collected. A conference dedicated to the exchange of experience in the education in polymer science in Russian universities has been organized. The collection of corresponding materials from the main European and American universities has commenced. Prof Khokhlov is planning to propose the organization of the Conference on Education in Polymer Science, to be jointly organised by IUPAC and European Polymer Federation, and to raise additional funding from UNESCO for this program.
- The MMD is also associated with the Interdivisional Committee on Nomenclature and Symbols (IDCNS), represented (A. D. Jenkins, Titular Member; K. Hatada, Associate Member; W. V. Metanomski, Secretary).

IUPAC COMMISSION IV.1

MACROMOLECULAR NOMENCLATURE

Since the General Assembly in Geneva, August 1997, the Commission has met from 19th – 22nd July, 1998, in Sydney, just after the World Polymer Congress, Macro '98. In addition, Professor R.G. Jones has organised a Working Party meeting in Mainz, connected with the Pool Project, 27/95.

PROJECTS

In the period covered by this report, the Commission has published TWO projects and worked on THIRTEEN other projects. W.V. Metanomski has also contributed, on behalf of the Commission, to Chapter 6 of the recent IUPAC publication *Principles of Chemical Nomenclature*. The number of projects published in this biennium is two less than for 1995 – 1997. However, several new projects were launched in Geneva and the number of active projects has increased by four. In addition, six new feasibility studies have been started.

Published Projects

1. (410/9/83) Source-Based Nomenclature for Non-Linear Macromolecules and Macromolecular Assemblies. *Pure & Appl. Chem.* 1997 **69** 2511-2521
2. (410/23/93) Terms Relating to the Non-Ultimate Mechanical Properties of Polymers. *Pure & Appl. Chem.* 1998 **70** 701-754

Current Projects

Liquid Crystals (410/18/87) Coordinator(s): V.P. Shibaev. A report has been prepared for public and IDCNS review by M. Barón, G. Luckhurst and R.F.T. Stepto. The reviews should be completed by 31st December, 1999.

Completion Date: 1997

Revision of Nomenclature of Regular, Single-Strand Polymers (410/19/89) Coordinator(s) J. Kahovec and W.V. Metanomski. This was discussed in Geneva and Sydney and is being prepared for public review

Completion Date: 1997

Generic Source-Based Nomenclature for Polymers (410/21/93) Coordinator(s) E. Maréchal. This was discussed in detail in Geneva and Sydney and a new version has been prepared by and circulated to the Commission. It will be discussed further by the Commission at the General Assembly in Berlin and prepared for public and IDCNS review shortly thereafter.

Completion Date: 1999

Guide to Polymer Terminology and Nomenclature (410/22/93) Coordinator(s) W.V. Metanomski. This was discussed in detail in Geneva and Sydney. Drafts of several chapters have now been completed and are under discussion. Further discussions will be held in Berlin. This project is a large undertaking. However, the structures of the chapters are taking shape and steady progress is being made.

Completion Date: 1999

Terminology Related to Multi-Phase Polymeric Composites and Blends (410/24/93) Coordinator(s) K. Horie and W.J. Work. A revised version has been prepared by W.J. Work since the Sydney meeting and is being distributed to outside experts. The project will be discussed further by the Commission at the General Assembly in Berlin.

Completion Date: 1999

Asymmetric Polymerizations (410/25/95) Coordinator(s) K. Hatada and J. Kahovec. The project was discussed in detail in Geneva and collaboration with Commission III.1 was established. A draft is being distributed to outside experts. The project will be discussed again by the Commission at the General Assembly in Berlin.

Completion Date: 2003

Kinetics and Thermodynamics of Polymerization (410/26/95) Coordinator(s) E. Maréchal and S. Penczek. A new draft was prepared by E. Maréchal and S. Penczek and discussed in Sydney. The assistance of R. G. Gilbert (Commission IV.2) was much appreciated. A new version is being prepared for distribution to outside experts and will be discussed by the Commission at the General Assembly in Berlin.

Completion Date: 2001

Terminology in Ceramics and Inorganic/Organic Polymeric Substances (410/27/95) Coordinator(s) R.G. Jones (Commission IV.1) and D. Holland, R.G. Jones (IV.1) has replaced A.B. Brennan (IV.1) as the Pool Titular Member directing the project. A list of terms was discussed at the meeting in Sydney and it was decided to amalgamate *Feasibility Study F-13 (Polymer Gel Terminology)* with the project. A Working party meeting was organized in Mainz by R.G. Jones, with M. Hess, I. Meisel and R.G. Jones attending. A new draft document will be discussed in Berlin. (D. Holland (II.2) the other Pool Titular Member no longer seems to be active on the project).

Completion Date: 2001

Terminology and Nomenclature of Hyperbranched Macromolecules and Dendrimer Molecules (410/28/97) Coordinator(s) J. Kahovec. This project was previously *Feasibility Study F-11*. It was launched as a new project in Geneva. A draft was prepared by J. Kahovec and E.S. Wilks for discussion in Sydney. A new draft will be prepared and discussed in Berlin.

Completion Date: 2003

Nomenclature of Cyclic Macromolecules (410/29/97) Coordinator(s) E. Maréchal. This project was *Feasibility Study F-12*. It was launched as a new project in Geneva. A draft was prepared by E. Maréchal for discussion in Sydney. It was decided that *Threaded Macrocylics* should be the subject of a separate study. (See *Feasibility Study F-20*.) A new draft will be prepared by E. Maréchal, R. Fox and E.S. Wilks for discussion in Berlin.

Completion Date: 2003

Glossary of Polymer Class Names (410/30/97) Coordinator(s) W.V. Metanomski. This project was previously *Feasibility Study F-14*. It was launched as a new project in Geneva. A draft was prepared by W.V. Metanomski for discussion in Sydney. A new draft will be prepared for discussion in Berlin.

Completion Date: 2003

Polymerization Processes and Polymers in Dispersed Systems (410/31/97) Coordinator(s) K. Horie, S. Penczek and S. Slomkowski. This project was initiated by S. Slomkowski with much international support. It was launched immediately as a project in Geneva. A draft was prepared by S. Slomkowski, S. Penczek and K. Horie for discussion in Sydney. A new draft will be prepared for discussion in Berlin.

Completion Date: 2003

Terminology of the Chromatography of Polymers and Related Materials.(422/1/98) This project is a collaborative project with Commission IV.2. It was launched in Geneva and is being coordinated by D. Berek of Commission IV.2. M. Hess is coordinating the activities of IV.1 on the project. A list of terms will be prepared by D. Berek and M. Hess for discussion in Berlin.

Completion Date: 2000

FEASIBILITY STUDIES

F-6 was proposed initially in Lisbon (1993), *F-13* in Seoul (1996), *F-15*, *F-16*, and *F-17* in Geneva and *F-18*, *F-19* and *F-20* in Sydney.

F-6: Thermal and Thermomechanical Properties of Polymers. Numerous letters of support for this project had been obtained and it was proposed in Sydney by R.G. Gilbert to make it a Division Project. This was agreed to and it was also agreed to involve the ICTA in the project. It would be prepared for launching as a project in Berlin.

F-13: Polymer Gel Terminology. The list of terms was discussed further in Sydney and it was decided to amalgamate the project with 27/95 on *Terminology in Ceramics and Inorganic/Organic Polymeric Substances*

F-15: Functionalization of Polymers. The list of terms to be considered was prepared by K. Horie for discussion in Sydney. Modifications were suggested. Letters of support were to be obtained and a draft prepared by K. Horie for discussion in Berlin, where, hopefully, it would be launched as a project.

F-16: Terminology of Ion-Containing Polymers. The proposed list of terms prepared by P. Kubisa was discussed in Sydney. Possible overlaps with Inorganic Chemistry nomenclature were discussed. Contacts would be made with the Inorganic Nomenclature Commission to define possible collaboration. A new draft with letters of support would be prepared by P. Kubisa for discussion in Berlin.

F-17: Terminology of Dielectric Properties of Polymers. A list of terms was prepared by M. Barón and discussed in Sydney. There was industrial support for the project but there appeared to be a lack of terms related specifically to polymers. Also, it may be desirable to include mechanical properties that are related to dielectric behaviour. A new list of terms and supporting letters would be prepared by M. Barón for discussion in Berlin.

F-18: Terminology Related to the Ultimate Mechanical Properties of Polymers. This project was proposed by W.J. Work. There was industrial support for the project, which would extend the Commission's recent publication on *Non-Ultimate Mechanical Properties*. A list of terms would be prepared by M. Hess, E.S. Wilks and W.J. Work for discussion in Berlin.

F-19: Source-Based Nomenclature for Modified Polymer Molecules. This project was proposed by E. Maréchal and E.S. Wilks. It is important for industry. A Working Party was formed; a list of terms would be prepared, and letters of support obtained, by E.S. Wilks for presentation and discussion in Berlin.

F-20: Nomenclature of Threaded Macrocyclic Molecules. This feasibility study arose from Project 29/97. A Working Party was formed; a list of terms would be prepared, and letters of support obtained, by E.S. Wilks for presentation and discussion in Berlin.

SUMMARY OF PROJECTS AND FEASIBILITY STUDIES

15 Projects, comprising:

2 projects published

- 1 project under IDCNS and public review
- 1 project being prepared for IDCNS and public review
- 9 projects under discussion by the Commission
- 1 pool-project under discussion by the Commission
- 1 project in collaboration with Commission IV.2

8 Feasibility Studies

OTHER ACTIVITIES

1. On-going revision of the Gold Book and IUPAC Database
2. Regular publication of the list of the Commission's publications and translations thereof in polymer journals
3. Establishment and maintenance of a World-Wide Web Page
4. Collaboration with the IUPAC Working Party on Student Nomenclature
5. Revision of the Purple Book
6. Preparation of a Comprehensive List of Terms, covering all of the Commission's recommendations.

R.F.T. Stepto

Chairman, IUPAC Commission IV.1

4th June 1999

Commission IV.2. Polymer Characterization and Properties

The Commission performs projects on the characterization and properties of polymers, through its working parties, that are of concern to the international polymer community, and which require input from this community. The structure of the Commission is based on a Commission Committee with its National representatives and Associate members, together with three Working Parties. The Commission has about 180 active scientists from Academe and Industry representing over 20 countries. The output and activities of the Commission over the last two years have been the publication of 12 papers.

The commission held a symposium in July, in Sydney 1998 with four aims.

- (i) *Review of all Commission projects (by the project coordinators or working party Chairs).*
- (ii) *Workshop on what our future scientific themes should be*
- (iii) *Commission structure and its future shape and form.*
- (iv) *Critical review of work.*

Working Party IV.2.1 “Structure and Properties of Commercial Plastics” (Dr H M Laun).

Current Projects

Melt Rheology and Concomitant Morphology in Polyblends and Polyalloys (421/15/86) Coordinator(s): A.P. Plochocki. Comprehensive experimental work completed. Draft publication for PAC in final revision.
Completion Date: 1996

Structure-Property Relationship of Discontinuous Fibre Reinforced Plastics (421/28/89). Coordinator(s): M. Bevis, A. Cervenka, and W. Gleissle. Final paper for PAC on rheology of reprocessed material in preparation.
Completion Date: 1999

Rubber Toughening of Plastics (421/29/91) Coordinator(s): C.B. Bucknall and M. Kozlowski. Experimental work close to completion. 2 papers for PAC in submission process. 1 paper published in J. Polym. Sci., 3 or 4 additional publications planned. 1997-8 publication: Mechanisms of cavitation over a range of temperatures in rubber-toughened PSAN containing three-stage core-shell particles by J.U.Starke, R.Godehardt, G.H.Michler and C.B.Bucknall, J. Mat. Sci., 22 (1997) 1855-1860.
Completion Date: 2001

The Influence of Reprocessing on the Structure-Property Characteristics of a Plasticised PVC Compound. (421/30/93) Coordinator(s): D.R. Moore and C. Dehennau. Experimental work completed. Draft publication for PAC available.
Completion Date: 2000

Structure and Properties of Hydrogenated NBR. (421/31/93) Coordinator(s): T. Kobatake and T. Masuda. Experimental work finished. 2 publications for PAC in preparation.
Completion Date: 1998

Characterization of finite length fibre composites: Part I. (421/32/95). Coordinator(s) D.R. Moore and A. Cervenka. Introductory paper by A.Cervenka and P.S.Allan, Pure & Appl. Chem. (1997) 1693-1705.
Completion Date: 2000

Characterization of finite length fibre composites: Part II. (421/32/95) Coordinator(s) D.R. Moore and A Cervenka. Mechanical performance of injection moulded composites: by L.Glas, P.S. Allan, T. Vu-Khjan and A. Cervenka, Pure & Appl. Chem.(1977) 1707-1723.
Completion Date: 2000

Characterization of finite length fibre composites: Part III. (421/32/95) Coordinator(s) D.R. Moore and A Cervenka. Studies on thin sections extracted from moldings (Wafers) by A.Cervenka and P.S.Allan, Pure & Appl. Chem. (1977) 1725-1740.
Completion Date: 2000

Characterization of finite length fibre composites. Part IV. (421/32/95) Coordinator(s) D.R. Moore and A. Cervenka. Structural studies on injection moulded composites by Bradsky, R.S.Bailey, A. Cervenka, G.Zachmann and P.S.Allan, Pure & Appl. Chem. 69 (1997) 2523-2539.
Completion Date: 2000

Characterization of finite length fibre composites: Part V. (421/32/95) Coordinator(s) D.R. Moore and A. Cervenka. Modelling of stiffness by P.S.Allan, A. Cervenka, and D.R. Moore, Pure & Appl.Chem. (1997) 1741-1751.
Completion Date: 2000

Characterization of finite length fibre composites. Part VI. (421/32/95) Coordinator(s) D.R. Moore and A. Cervenka. Rheological studies of materials based on the PP matrix by R.S.Bailey and D.J.Groves, Pure & Appl. Chem. 69 (1997) 2541-2565.

Future Requirements in the Characterization of Continuous Fibre Reinforced Polymeric Composites. (421/32/95). Coordinator(s): D.R. Moore and A. Cervenka. 1 paper for PAC planned. Drafts of chapters available.
Completion Date: 2000

Rheological and Mechanical Properties of P-alpha-MSAN/PMMA Blends in Miscible and Phase Separated Regimes of Various Morphologies. (421/33/95) Coordinators: H.M. Laun, L. Lyngaae-Jørgensen and V. Altstädt. Experimental work on rheology close to completion. Experiments on mechanical properties ongoing. Efforts are undertaken to provide the complete phase diagram. Rheological and mechanical properties of poly(alpha-methylstyrene-co-acrylonitrile)/poly(methyl methacrylate) blends in miscible and phase separated regimes of various morphologies. Part 1. Characterization of constituents, blend preparation, and overview on blend morphology. Pure & Appl. Chem. 70 (1998) 1547-1566. Rheological and mechanical properties of P-alpha-MSAN/PMMA blends in miscible and phase separated regimes of various morphologies. Part 2. Limits of miscibility in the quiescent state and during flow" by V. Schytt and J. Lyngaae-Jørgensen, Polym.Networks blends 7 (1997) 77-86. Four additional publications planned.
Completion Date: 2001

Property Improvement via Interfacial Chemical Reaction - Reactive Extrusion of EVOH/SMA and Polyamide/MAH-EPR. (421/34/95) Coordinator(s): J.E. Curry, J.G. Bonner, and P.S. Hope. Experimental work on Nylon 12/MAH-g-EPR ongoing. Second paper for PAC planned concerned with the mechanical properties. A collaborative study of the structure and rheological properties of EVOH/SMA blends produced by reaction extrusion by P.S. Hope, J.G. Bonner and J.E. Curry, Pure & Appl.Chem., 68 (1996) 1665-1685
Completion Date: 2001

Effects of Side-Chain Branching on Processability of Commercial Polycarbonates. (421/35/97) Coordinator(s): M. Takahashi, K. Sato, T. Masuda. Samples distributed and experimental work ongoing. 1 or 2 papers for PAC planned.
Completion Date: 2000

Studies on Biodegradable Poly(epsilon-caprolactone) (421/36/97) Coordinator(s): M. Hirami, M. Mochizuki, T. Hayashi. Experimental work almost finished. Second paper for PAC in preparation. Studies on biodegradable poly(hexano-6-lactone) fibres. 1. Structure and properties of drawn poly(hexano-6-lactone) fibres by M.Mochizuki, K. Nakayama, R. Qian, B.-Z. Jiang, M.Hirami, T.Hayashi, T.Masuda, and A.Nakajima, Pure & Appl. Chem. 69 (1997) 2567-2575.
Completion Date: 1999

Working Party IV.2.2 "Molecular Characterization of Commercial Plastics" (Dr D Berek)

Activities were restarted in 1996. Six projects were proposed and accepted at the General Assembly in Geneva in August 1997. The Working Party has 38 members with participation from 14 different countries.

Nomenclature of chromatography of polymers and related substances. (422/1/98) Coordinator(s): D. Berek. No reports yet available.
Completion Date: 2000

Characterization of polyelectrolytes in aqueous solution by GPC, light scattering, viscometry, ultracentrifuge or similar methods. (422/2/98) Coordinator(s): R. Bruessau. First round is finished and the publication is under preparation.
Completion Date: 2000

Size exclusion chromatography dispersion correction. (422/3/98) Coordinator(s): M. Potschka. No reports yet available.
Completion Date: 2000

Precise determination of molecular weight distributions of polyolefins by high temperature size exclusion chromatography and hyphenated techniques. (422/4/98) Coordinator(s): D. Lilje. No reports yet available.
Completion Date: 2000

EC/GPC of polystyrenes. (422/5/98) Coordinator(s): S. Mori. First round completed. No reports yet available.
Completion Date: 2000

Molecular characterization of polyamides 6, 11 and 12.(422/6/98) Coordinator(s): E. Robert. 2/2 First round was finished and the publication is under preparation.
Completion Date: 2000

Working Party IV.2.8 “Modelling of Polymerization Kinetics and Processes” (Prof M Buback)

Critically Evaluated Database of Kinetic Parameters for Free-Radical Polymerization (410/3/99)
This working party has 38 members and one project on the critical evaluated database of kinetic parameters for free radical polymerization. Recent activities have focused on pulsed laser polymerization and to use these methods to “benchmark” other methods.

(A) Papers 1997-9

1.S. Beuermann, M. Buback, R.G. Gilbert, R.A. Hutchinson, B. Klumpermann, F.O. Olaj, G.T. Russell, J. Schweer, *Macromol. Chem. Phys.*, **198**, 1545 (1997). “Critically evaluated rate coefficients for free-radical polymerization, 2. Propagation rate coefficients for methyl methacrylate”

2. *Pure and Applied Chemistry* 70, 1415-1418 (1998)

"Critically-evaluated propagation rate coefficients in free radical polymerizations -II. Alkyl methacrylates", S. Beuermann, M. Buback.

3. "Critically evaluated rate coefficients for free-radical polymerization 3, Propagation rate coefficients for Alkyl Methacrylates", to be discussed and finalized before and at the ACS Meeting, New Orleans, August 1999

Papers to be prepared in the near future (the experimental material is already available):

3. "Critically evaluated rate coefficients in free-radical polymerization 4, Propagation rate coefficients of Functional Methacrylates"

4. "Critically evaluated rate coefficients in free-radical polymerization 5, Propagation rate coefficients for Acrylates"

(B) Working Party Meetings since Geneva

Gold Coast (IUPAC Macro 98), Australia, July 12, 1998; New Orleans (ACS Meeting), USA, August 21, 1999

(C) Ongoing work and planned future projects:

- Propagation rate coefficients for free-radical copolymerizations
- Termination rate coefficients in free-radical polymerizations - Critical evaluation of methods and results
- Termination rate coefficients in free-radical copolymerizations - Critical evaluation of methods and results
- Chain - transfer rate coefficients in free-radical polymerizations - Critical evaluation of methods and results:
- Chain transfer to monomer, chain transfer to chain-transfer agents
- Initiator decomposition rates

(4) Further activities:

An SEC assembly has been installed at the Slovak Academy of Science, run by I. Lacik. Funding has been obtained from Volkswagen-Stiftung. PLP-SEC studies into propagation rate coefficients have been started in Jean-Pierre Vairon's group in Paris. Having now several places in the world available for this kind of analysis is extremely valuable for the intentions of our IUPAC WP activities. It should also be mentioned that from joint efforts within the WP (colleagues from the groups of Gilbert and van Herk both working at Kamachi's lab), the discrepancies in data from PLP-SEC and ESR are now better understood and consistent data have been obtained for the systems that were recently studied.

Commission IV.3. Functional Polymers

Projects:

Working party on "Recycling of Polymers" (Chairman: Dr. Norbert Bikales)

The working party presented its final report at the IUPAC MMD meeting in Geneva, August 1997. The recommendations were unanimously approved, so that this working party has accomplished its assigned task. Publication: *Macromol. Symp.* **135**, 287-94 (1998).

Working party on “*Biodegradable Polymers*” (Chair: Prof. Anne-Christine Albertsson). 430/5/93
Biodegradable Polymers Coordinator(s): A.C. Albertsson and S. Huang. The most recent activity
and meeting took place in the context of the 5th International Scientific Workshop on
“Biodegradable Plastics and Polymers”, June 9-13, 1998 in Stockholm. No report available.
Completion Date: 1997