IUPAC Working Party IV.2.1

"STRUCTURE AND PROPERTIES OF COMMERCIAL POLYMERS"

Meeting No. 61
Held at the Stonefield Castle, Tarbert, Scotland
1st to 3rd October, 2003

Hosted by Rob Bailey and Dave Stocks, ICI Measurement Science Group, UK.

Chairman: Dr. H.M. Laun, BASF, Germany.
Secretary: Dr. R.S. Bailey, ICI, UK.

Narrative:

This meeting was well attended with 27 attendees.

This meeting was held in an unusual location, which gave the working party (soon to be an IUPAC subcommittee) the chance to celebrate the 40th anniversary of the working party. ICI Measurement Science Group hosted the banquet for this occasion.

The website can be found on www.launweb.de/iupac. It will be continuously updated and will contain all relevant reference material relating to our Working Party activities and will become the focal point of our communication in future.
LIST OF ATTENDANCE

Working Party Members:

Altstaedt, Prof. V. UNIVERSITAT BAYREUTH Germany
Bailey, Dr. R.S. (WP Secretary)ICI UK
Bucknall, Prof. C. CRANFIELD UNIVERSITY UK
Chai, Dr. C. BP LAVERA France
Covas, Dr. J. UNIVERSIDADE DO MINHO Portugal
Dijkstra, Dr. D. BAYER Germany
De Vries, Dr. S Dow Benelux
Gunesin, Dr. B. DUTOIT-GUNESIS Switzerland
Handge, Dr. U. ETH ZURICH Switzerland
Inoue, Prof. T. KYOTO UNIVERSITY Japan
Kim, Prof. S.-C., KAIST Korea
Kaszas, Dr. G. BAYER Canada
Lambert, P ICI UK
Langouche, Dr. F. SOLVAY Belgium
Laun, Dr. H-M (WP Chairman) BASF Germany
Lauterbach, A ICI/BAYREUTH Germany
Mangnus, Dr. M. Dow Benelux
McNicol, Dr. A. ICI UK
Puskas, Prof. J. UWO LONDON/Akron Canada/USA
Ruellmann, Dr. M. BASF Germany
Steininger, Dr. H. BASF Germany
Stocks, Mr. D. ICI UK
Wassner, Dr. E. ELASTOGRAIN Germany
Zoetelief, Dr. W. DSM Germany

Observers:

Robinson, Dr. I. LUCITE INTERNATIONAL UK
Minutes of Meeting 61 held in Tarbert, Scotland.

1st October to 3rd October 2003

ADMINISTRATIVE ITEMS

1. Opening, introduction of participants and finalisation of agenda

The chairman welcomed all Working Party (WP) members and observers.

The agenda was outlined and agreed.

Each participant introduced themselves.

The minutes of meeting 60 in Canada was approved. The minutes for Ludwigshafen meeting (60b) will be approved at the next meeting. Laun outlined the mode of operation of the working party (outlined on the WP website). For the observers and new IUPAC WP representatives from industry, the operation of IUPAC was outlined. The chairman suggested the Ludwigshafen meeting was to be renamed meeting 61a since the EA meeting was cancelled due to the SARS outbreak.

Apologies for absence were received from all active members who were not able to attend. 27 members and observers attended the meeting.

2. Rules and Membership

The present list of WP members and their addresses are now maintained on the Working Party website. REMINDER: www.launweb.de/iupac. Access to the private sector is (username: iupac     password: iupac). It is updated after each WP meeting, but please send any changes to your personal details directly to the WP Secretary by e-mail: (dick.dijkstra@bayerpolymers.com)

The Working Party rules are also now available on the website.

Membership changes and actions:

The Secretary has written to the following to encourage a strong positive response to indicate future active participation:-
Covas, Szewczek, Plochocki, Aras.
As a result of this, Covas attended this meeting, but the others will no longer participate.

Ideas for new members who would be active are encouraged. Please send a contact e-mail address to the Secretary.
Laun reviewed the content of the website – and is looking for an academic who could update the citation index (Handge kindly offered to do this).

To reiterate the membership rules.
1) All communication is to be made electronically. It is a requirement of each member to make their current working e-mail address available.
2) Details of the meeting are distributed on the website.
3) Alert messages from the secretary are to be sent out when important changes are made to the website.
4) Reports and reprints of papers arising from the output should be made available on the website (through the chairman or secretary) as .pdf or Powerpoint files.

Laun wishes to stand down as the chairman this year after 9 years service. Bailey is willing to stand as the new chairman and Dijkstra as the new Secretary. Puskas seconded the proposal. Other proposals were invited and an election of officers took place. There were no other nominees and so the new officers will be Bailey and the Secretary will be Dijkstra. This was passed unanimously.

Report from the MMD meeting.
Laun described the IUPAC General Assembly held this August in Ottawa, Canada. The Working Party activity that has taken place as a consequence of the clearing of the old pre-SDIC projects was presented. This has resulted in 16 papers. The summary of this is available on the website (private section). An overview of the old projects was also given, the titles of the publications and the status is given on the private sector of the website.

The Ottawa GA was attended by Laun, Kim and Bailey. Laun showed the materials that were presented and these are shown in the private sector on the website.
The paper describing the history of the WP will be condensed into a 2 page document. 80 papers have been written over the years.

Laun has now stood down as Characterisation coordinator, but Kim was voted in as a Titular member and Bailey as an Associate member for the future meetings. The response at the Division meeting was very positive. The President of the MMD had hoped to attend our meeting in Scotland but was unavoidably detained. At the Ottawa meeting the move to allow WPIV.2.1 to become a working sub-committee was agreed and this step will take place as from 1st January 2004. This would help to make the WP activities visible in the IUPAC organisation. Furthermore, the WP activities and members will be listed in the IUPAC Blue Book. The old nomenclature activity (now called Terminology) has become a sub-committee. In the bylaws, the sub-committee has a limited lifetime of 2 years (which is much shorter than the projects), but this will be renewed more or less automatically at MMD meetings. Stepto guarantees that renewal of sub-committee status will be automatic if it is active. Bailey and Kim (as co-chairman) and Dijkstra and Lee (as co-secretaries) was the structure proposed in order to be able to make the transition to a sub-committee. This will be published in the IUPAC blue book.
New projects are encouraged – especially in the area of education.
Laun has arranged for the website to be transferred to the official IUPAC website. A CD was sent to Fabienne Meyers (at IUPAC)
Kim presented an update of the East Asian activities. A meeting was planned in August but because of SARS this was cancelled. There are two running projects, Structure and Properties of Cyclic Olefin Copolymers. He gave the status showing the 3 papers in preparation. (see paper copy from Kim). The second project Structure and Properties of Polyester Elastomers composed of PBT and PCL. This just started this year. The project is still open for participation. The materials are supplied by Toyobo, the materials are distributed and available. Please contact Prof. Takagawa in Kyoto University if you wish to participate.

The next IUPAC General Assembly will be in Brazil. Meetings of the MMD are scheduled for the MACRO meeting in Paris in 2004, this is also our proposal for our next (subcommittee on Structure and Properties of Commercial Polymers) meeting.

**Tactical planning for projects.**
New projects remain under the WP control while they are feasibility projects, once they become an official IUPAC MMD project they are subject to 3 years and a tight deadline.

**Dates of future meetings of WP IV.2.1**
The next Working Party meetings are tentatively arranged as follows:

<table>
<thead>
<tr>
<th>meeting number</th>
<th>date</th>
<th>Venue</th>
<th>host/comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>61a</td>
<td>4th Aug. 2003</td>
<td>Seoul, Korea</td>
<td>Prof. K. C. Kim</td>
</tr>
<tr>
<td></td>
<td>18 to 20 September 2003</td>
<td>Intern. Polymer Symposium, Kyungju, Korea.</td>
<td></td>
</tr>
<tr>
<td>62</td>
<td>July 1 – 2, 2004</td>
<td>Palais de Congres, Paris</td>
<td>IUPAC organisation (J.-P. Veron is the contact)</td>
</tr>
<tr>
<td></td>
<td>July 4 – 9, 2004</td>
<td>(joint meeting with our EA colleagues)</td>
<td>(in line with IUPAC World Polymer Congress - MACRO conference and MMD meeting)</td>
</tr>
<tr>
<td>62a</td>
<td>2004</td>
<td>EA Research meeting in Japan (to be decided)</td>
<td></td>
</tr>
<tr>
<td>63/64</td>
<td>2005/2006</td>
<td>Invitations welcome</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>Bayer and DSM have offered to host a meeting. Also, Budapest Hungary in 2006. Akron USA has also been mentioned.</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>2006 MACRO will be in Rio de Janeiro, Brazil.</td>
<td></td>
</tr>
</tbody>
</table>
Future meetings can be arranged to provide one and a half days for discussion or more depending on the organisers discretion.

It is intended to invite observers from major companies which are not yet represented in the WP.

**New Members**
Observers who attended decided as follows:-

Dr. Ian Robinson – yes, he will become a provisional member. Lucite International will become a full industrial member if Ian is actively involved over 2 years.

**Any other business.**

Format of the meeting. It is still not necessary to have separate rheology and mechanical sessions. These may become valuable again in the future.

International representation is limited now. Some countries (Ireland, France, Scandanavia, Africa, Americas) are not available. Laun is aiming to include Nicholson (Sydney) in the activities of the WP. He may join this group or the East Asian working group.
6. Reviews and discussion on running IUPAC projects

All project details are now being set up so that they in a web compatible format. WP members should look at the website and Project Co-ordinators should update their project details by sending updated text to the WP Chairman who will arrange for the appropriate web pages to be updated. Consequently only a brief progress summary and an action list will follow an executive summary of the technical aims, theme and publications.

[Note: the projects which are in grey have been completed and there are no further actions required. Those in black text still have some outstanding issues.]

Project # 421/15/86
Title: Melt Rheology and Concomitant Morphology in Polyblends and Polyalloys
Co-ordinator(s): A.P. Plochocki
Completion Date: 2002

Status: This project is now complete. A publication has been submitted to PAC. [“Melt rheology and concomitant morphology of model binary mixture of polyethylene and polystyrene (polyblend)”.] Laun will complete this and address the issues raised by PAC.

Project # 421/20/87
Title: Characterisation of flow behaviour and properties of Liquid Crystal and Aromatic Polymers
Co-ordinator(s): J White
Completion date: 2002

Status: This project is now complete. A publication has been submitted to PAC but needs revision after the review process. [“The rheological properties and associated structural characteristics of some aromatic polycondensates including liquid crystalline polyesters and cellulose derivatives”].

Project # 421/28/89
Title: Structure-Property Relationship of Discontinuous Fibre Reinforced Plastics
Co-ordinator(s): M. Bevis, A. Cervenka, and W. Gleissle
Completion Date: 2001

Status: This project is now complete. 7 publications have been issued.

Project # 421/29/91
Title: Rubber Toughening of Plastics
Co-ordinator(s): C.B. Bucknall and M. Kozlowski
Completion Date: 2001

Status: This project is almost complete. 4 publications have already been issued. Part 5 was circulated – comments are invited – Bucknall will contact Ausimont to see if they wish to co-author. Gray has now left BP and Chai will approve the content of the paper. Paper 4, is still being finalised (with Altstaedt). Heckman is being consulted. The aim is for this publication to be completed within the next few months.

Project # 421/30/93
Title: The Influence of Reprocessing on the Structure-Property Characteristics of a Plasticised PVC Compound
Co-ordinator(s): D. R. Moore and C. Dehennau
Completion Date: 2000

Status: This project is completed and the paper issued. [“The influence of reprocessing on the structure-property characterisation of a plasticised PVC compound”].
Project # 421/31/93  
Title: Structure and Properties of Hydrogenated NBR  
Co-ordinator(s): T. Kobatake and T. Masuda  
Completion Date: 2002  

Status: Project complete. 2 papers will be submitted to PAC. Kim will check the status of this project.

Project # 421/32/95  
Title: Future Requirements in the Characterisation of Continuous Fibre Reinforced Polymeric Composites  
Coordinator(s): D.R. Moore and A. Cervenka  
Completion Date: 2002  

Status: This project is completed.

Project # 421/33/95  
Title: Rheological and Mechanical Properties of P-alpha-MSAN/PMMA Blends in Miscible and Phase Separated Regimes of Various Morphologies  
Coordinator(s): H.M. Laun, L. Lyngaae-Jörgensen and V. Altstädt  
Completion Date: 2002  

Status: This project is complete with an impressive 11 publications in total.

Project # 421/34/95  
Title: Property Improvement via Interfacial Chemical Reaction - Reactive Extrusion of EVOH/SMA and Polyamide/MAH-EPR  
Co-ordinator(s): J.E. Curry, J.G. Bonner, and P.S. Hope  
Completion Date: 2001  

Status: This project is now complete. 2 papers have been published in PAC.

Project # 421/35/97  
Title: Effects of Side-Chain Branching on Processability of Commercial Polycarbonates  
Co-ordinator(s): M. Takahashi, K. Sato, T. Masuda  
Completion Date: 2002  

Status: This project is complete. 2 publications will be submitted to PAC. Manuscripts not yet available. Kim will check the status of these manuscripts.

Project # 421/36/97  
Title: Studies on Biodegradable Poly(ε-caprolactone) fibres.  
Co-ordinator(s): M. Hirami, M. Mochizuki, T. Hayashi  
Completion Date: 2001  

Status: Project completed with 3 publications now available in PAC.

Concluding comments regarding pre-SDIC projects.

All projects have been completed. Some few publications are still in the submission process.
Official full projects (since Berlin General Assembly)

Project # 421/37/99
Title: Quantifying scratch resistance of commercial polymers
Task Group Leader: R. Bailey, J Puskas.
Completion date: 2005

Progress:
Stage 1
Bailey reviewed the status of the project plan. There are 2 parts to this project. A great deal of work has gone into sourcing and distributing materials for this project this year. However it now seems clear that the project will be completed with data generated from the limited successful materials. There is enough data for publications to be made. Presentations were made by Lambert, Lauterbach and McNicol (all from ICI), on the phase 1 part of the project.
There is enough material to produce at least one paper. It was proposed that two papers on scratch resistance techniques for commercial plastics. The first would be on single asperity contacts (scratching) and the second on multi-asperity contacts (abrasion). It is hoped that these could be presented at a conference soon, and the papers will be prepared and available for comments for the next IUPAC meeting in Paris.

Stage 2:
Materials have been offered for the second part of the project.
Puskas will outline the project plan next year in Paris.

Project # 421/38/00
Title: Structure and Properties of Cyclic Olefin Copolymers
Task Group Leader: S.C. Kim, KAIST; T. Takigawa (Kyoto)
Completion date: 2003

Kim presented new work. A Powerpoint presentation (available on the website) was given. 2 papers have been prepared. A further publication will be completed by the end of 2003. Two further papers are expected in 2004.

4 publications are planned:-
1. Chemical structure and physical properties by Kim, He and Jiang. (publications sent to Laun already).
2. Optical properties by Inoue.
3. Mechanical and dynamic mechanical properties by Nitta, Nakayama and Michler.
4. Rheological properties by Takigawa, Dijkstra and He.

Project # 421/39/02
Title: Structure and Properties of polyester elastomers composed of poly(butylenes terephthalate) and poly(e-caprolactone)
Completion date: end of 2005 (starting 1st Jan 2003)

The project was approved last year and is now a full running project. However a detailed progress update was not available.
There are 5 sub topics
- molecular structure
- rheological properties
- rubber elasticity
- aggregate structure and deformation mechanisms.
- Blends with other polymers
- Degradation (this topic is now not taking place).

Takagawa has invited contributions from this working party. More polymers are also invited.

**Project # 421/40/03**

**Title:** Recommendations for data presentation applicable to mechanical and rheological measurements of polymers.


Now approved and started in April 2003.

Wassner reviewed the scope of the project. The aim of the project is to convince the instrument manufacturers to improve the current state of instrument software and to participate.

Wassner aims to complete recommendations and best practice examples based on accepted practice for October 2003. Only a few labs have done this to ISO 6721.

Next milestone is to invite and discuss the rheometer manufacturers, this is not likely to be well attended by the instrument manufacturers since they are not enjoying a good level of business. After this meeting Wassner will write a letter to the manufacturers – and needs all members to help, to indicate the breadth of interest across industry and academia.

16 members indicated interest at Ludwigshafen.

What will be done to influence the instrument manufacturers? This has to be done in concert by our members who hold some influence over these manufacturers, and should collaborate to get attention from instrument suppliers.

Is a separate meeting needed? It may be premature to do that now.

Recommendations are needed and a document could be produced.

The advantages of doing this for some example data (from an IUPAC project) should be used which illustrates the case for this on selected instruments. Participants will receive the document and act within a limited time scale.

A new version of a downloadable Excel Macro will be made available on our website. Iris compatibility will also be addressed for relaxation spectra calculation. We can invite or inform this contact through Laun. Wassner will also circulate the macro to participants by email. A deadline for response will be given. Mention should be made that this comes from an official subcommittee of IUPAC.

**7. Reviews and discussion on running Feasibility studies**

Laun pointed out that there was a need to review which of the 9 feasibility studies can be transferred into full project proposals.

**Feasibility study 3**

**Title:** Structure and Properties of linear and crosslinked structural PVC foams.

Co-ordinators: V. Altstaedt and A. Cervenka.

Progress:-

Altstaedt gave background to the new project. In September, a full project proposal was made to IUPAC.

Altstaedt needs to revise the form to reflect himself as the task group leader. The budget should also be increased to $3000. The proposal form will be distributed to all MMD members. Bob Steptoe should be informed that the form needs to be updated.

3 papers will be suggested. The first paper (based on the feasibility project) another on fracture mechanics, the final on shear behaviour.

Many of the list of contributors have left and need to be updated.

Altstaedt stressed the importance of foamed materials. A linear and a crosslinked PVC foams have been obtained.
Altstaedt will check with Cervenka to see if he is still wishing to be co-coordinator of the project.
Dijkstra and Steininger have issued reports. More contributions are needed.
DMA measurements were offered by Wassner, Steininger and Bucknall. Kaszas offered to do chemical analysis.
Some samples from inactive members need to be retrieved. Laun urged Altstaedt to define a list of specific task. Perhaps East Asian members would like to contribute?

**Feasibility study 4**
**Title: What makes thermoplastic vulcanizates (TPV) such versatile materials?**
**Co-ordinator: B. Gunesin & A. Galeski**

**Progress:**
Gunesin presented the status of the work. It is likely that this will not become a full project but there is enough data for a publication. The two formulations soft (64) and hard (40) have been studied but the composition is still not clear. Laun’s old rheology data was revisited following discussion with Coran. Zoetelief pointed out that this is typical behaviour, but Laun can repeat the data with differing dwell times. More morphology data is requested on orientation and Gunesin will pursue collaborators.

The plan is to have a rheology paper and then a solid state properties in the beginning of 2004. This will be completed as a feasibility study.
Feasibility project 6
Title: Flow properties of ceramic and metal injection moulding feed stocks
Proposer: W. Gleissle/B. Hochstein and H. M. Laun

Progress:
Laun reviewed the project aims. BASF Catamold® materials are available (POM matrix).
There are 3 parts to the project. The first of these is capillary rheometer activities.
Catamold granules are injection moulded to form a green body. By acid etching debinding
gives a component which is subsequently sintered.
The latest work was reviewed, with sharkskin and dragons teeth effects, negative wall slip
effects. BASF used an automated nitrogen capillary rheometer to study these machines. This
allows very precise measurements in the low pressure region. The effective wall shear rate
was calculated from the Mooney plot. Further hydrostatic pressure measurements using a
throttle design die. Inlet and external pressure transducers add-on for Gottfert rheograph. The
pressure drop as a function of external pressure is plotted, to give a throttle pressure
dependence coefficient.
Laun encouraged everyone to participate. Slit dies work is needed. Slip velocity is needed,
(see webpage for the detailed aspects of the 3 parts of the tactical plan). Zoetelief will help with
the slit die measurements. Langouche is also offering to help with throttling studies.
Is there any interest from the East Asian research group?
Laun will make a list of the contributions required and contact all the other WP members.

Feasibility study 9
Title: A critical check of viscoelastic capillary flow predictions using viscoelastic finite
element simulation and IUPAC LDPE literature data.
Co-ordinator: H. M. Laun and D. Dijkstra.

Progress:
Contact has been made with Nicholson (ex-Leeds now at Sydney) and Mitsoulis. The meshes
and data have been defined now and the simulations have been run for 3 defined geometries.
Laun showed the improvement in the fit for extrusion contours with slight data refinements
from old (1970) to new data. Following Ourieva’s suggestion at Ludwigshafen an annular die
has been investigated (using a 2D simulation).

There are now 2 parts:
FEM simulation: circular dies, annular dies.
Experiments: contour of extrudates from circular dies, contour of extrudates from annular dies.
The materials set could be expanded using polystyrene for example.
Covas can help with finite volume studies, Dow can also help. Laun will send out a request
form to solicit interest, materials required and suggested new measurements. Some
participants have not yet received the data files yet (i.e. Zoetelief). Mangnus would also like to
contribute. Chai will help on HDPE.

Feasibility study 10
Title: The role of stress-induced cavitation in the mechanical performance of semi-
crystalline polymers.
Co-ordinator: A. Galeski and C. Bucknall.

No progress has been made. Bucknall will contact Galeski and is happy to continue work on
this project. Please contact either coordinator with ideas or offer of help.

Feasibility study 11
Title: Rheological characterisation of polyamides.
Co-ordinator: D. Dijkstra and W. Zoetelief.

Polyamide 6 (Durethan B30S) results (materials have been partially distributed) were shown by
Laun (ARES) and he showed drying of up to 7 days is needed. Overdrying is continued in the
rheometer and the effect of polycondensation increasing the viscosity is shown. Over 4
decades of angular velocity data looks consistent across ARES and PRV measurements. Zoetelief also looked at a number of drying regimes, prior to rheological measurements. He showed a range of moisture contents all gave differing polycondensation as expected, and capillary rheometry data also showed a broad range of behaviour. The observations between torsional data and capillary data do contradict.

Koopmans’ results were also presented. Some further interpretation is needed. Dijkstra showed data from Bayer, illustrating the stability issues and the lack of convergence to a mastercurve at higher temperatures. Measurements at different samples can give a different activation energy (Laun) and so these measurements must be accompanied by a molecular weight analysis.

For future work a reference temperature will be given. Another idea is for the new chairman of the molecular characterisation subcommittee is to be approached and to carry out some comparison measurements. Solution viscometry and GPC should be undertaken. Zoetelief suggests that a molecular weight might vary across the plate radius, since there is a plate diameter dependence. Could this be corrected for?

High frequency equipment (Mettler Toledo DMA) was used in shear at Bayer. The correlation between ARES or Mettler converge (for the same residence time) is good at 230°C but as temperature increase (10°C steps) the two techniques correlate less well. Is the moisture control as good in the Mettler instrument? The oscillatory shear measurements were compared with capillary data. Cox Merz clearly doesn’t apply as the temperature increases.

At this stage the conclusion can be made that this is a very worthwhile project and the difficulties in characterising these materials is real.

A reference temperature (240°C?) is needed. All samples should be kept. Before and after testing.

Laun believes considers that the project should concentrate on polyamide 6. At first additive free polymer, then with additives and the caprolactone

Should this be a full project? Materials, challenges and contributors are already defined. Dijkstra can start to fill out the form!

A questionnaire could be circulated in which the contributions and the amount of material needed would be collected. This could be collated into a tactical plan.

Feasibility study 12
Title: Future developments of new materials based on commodity polymers by physical structure and morphology alteration.
Co-ordinator: A. Galeski and C. Bucknall.

The manuscript for the history feasibility study is now available on the website. A volunteer is needed for someone to check the citation index of for the 80 papers. Ulrich Handge will do this.

A shortened version will be available. This will be published in PAC and so will be downloadable (free) as .pdf files from the IUPAC server. [this is one big positive motivation for using Pure and Applied Chemistry].

8. NEW FULL PROJECT PROPOSALS to be submitted to IUPAC

Techniques to study commercial nano composites based on organic clays.
Proposer: S. C. Kim and J. Lyngaae-Jorgensen

TPO clay nano composites are being explored in GM, nylon 6 nanocomposite Ube Industries for a timing belt cover application. AIM Barrier property advantages in packaging products. High barrier film & coatings – whilst retaining transparency. (Honeywell, Bayer with nylon NXD6) Mitsubishi Gas chemical and Eastman. Also imparts mechanical properties with 1 or 2% clay with exfoliated structure.
Clay sheets mixing issues with polymers. Kim showed list of interested companies. Other matrix polymers include PP, unsaturated polyester, UHMWPE, PBT, PETG, PPS, PC. Also Lucite PMMA is included from Robinson (agreed at this meeting). Bayer, Clariant, Honeywell, Eastman, RTP, Unitika, Ube are all participating in the project.

Melt blending
Resulting in 1. Tactoid, 2. Intercalated (some chains penetrating into the gallery of the clay), expanded distance between the sheets marginally. 3. Incalated disordered (some breakage of the clay and the sheets are disrupted and misaligned relative to one another). 4. Fully separated 'exfoliated' or delaminated – this is the final goal.

For commercial products – there may be a mixture of these.

Project proposal available from Kim (circulated at the meeting).

Robinson will participate (materials supply). Dijkstra will also. Chai will contribute measurement, Laun – rheology measurements & permeation. Links with the PA6 characterisation, Covas will rheology and processability, Mangnus offered elongational rheology. Langouche will also help with rheology. Zoetelief will help with mechanical properties, rheology and permeability.

For mechanical properties (and permeability), compression moulded plaques will be provided (Kim will investigate this). Neat PA6 and PMMA will also be available.

Proposal for IUPAC will be circulated to Bailey for the minutes.
Laun will put the background slides on the web.

2. The foams project (Altstaedt) will be submitted

3. The polyamide 6 characterisation project (Dijkstra).
6. New project proposals

On the theme of Education.

**A polymer processing tutorial.**

Proposer: Laun

Education materials could be made available for education purposes. A presentation could be made available to the Education coordinator (Ron Sanderson) for developing countries. (this would be the focus and via the internet). Laun encouraged ideas on this theme.

Bucknall would like to see a guide to the software (review of what’s available) for modelling processing. Is this group the right group? This is not covered in the text books or literature. This is a sub-project of Laun’s original idea. Altstaedt suggests this could be on the webpage – as a communication, with teaching materials. Puskas pointed out that it is the material in combination with the credibility of individuals in industry or academe that would be valued.

A movie would be ideal. Chai suggest 2 levels – basic materials (as a Powerpoint presentation) and actual material presented in video form.

Kim challenged whether this fits with this body as Structure Properties or classification of commercial polymers.

De Vries suggested that a Campus based database system in the Dow intranet that could be included or made more publically available.

The revised title was proposed for this project as:-- **Structure and Properties of commercial polymers tutorial.**

The requirement for this will be checked by Laun. He will contact Ron Sanderson. Laun will propose a more detailed project for the next meeting. In Paris, it may be possible to explore what the requirements are for this and to meet some of the educators in the developing countries.

Puskas offered to collect some examples (Dow, Bayer, BASF) of industrial in preparation for the Paris meeting.

**Microstructural, rheological and mechanical properties of (un)compatible PA6/ABS blends with and without compatibilisers.** (materials from BASF).

Proposer: Handge

This would be a systematic analysis in the influence of compatibilisers (some theoretical approaches. This includes microstructure/rheology/mechanical/theoretical contributions. These materials are used for toughening nylon for laptop computer cases. These are commercial products. Bayer may also have an PC/ABS blends in similar applications.

Blending/compatibilising would be done by the suppliers. The subsequent processing (compression moulding) materials will need to fixed during the feasibility study. A new blends project is proposed following the completion of the earlier blends. The influence of the interfacial tension on the properties can be assessed (with and without compatibilisers). What would be the main variables (concentration of the phases; compatibiliser; dispersion (discreet or co-continuous phases?)). The compatibilisers will be disclosed. The final objective of the project – is to understand the influence of the variables.

This is a complex subject and the project is very complicated. BASF do not want to disclose the full compositional details of their commercial blends.

There can be some overlap (synergism) with the proposed PA6 project.

Handge will check the sample preparation with BASF.

**Critical check of Fourier Transform rheology.**

Proposer: Mangnus

The focus of this proposal would be to consider the Pros and cons of this technique. There are limitations of the technique in various fields. Also limited numbers of labs have this technique. Could it be compared with the multiwave data available on other rheometers?
Since there are a limited possible participants Christian Bailey (alpha technologies), Christian Freidrich (Freiberg), Dr. Wilhelm (reinventor) of the technique could be invited to participate. Dealy could also be invited.

A champion for this project is needed with a view to working up a proposal for the next meeting.

Laun believes a position paper could be useful.

Mangnus (and/or his colleague Koopmans) will come up with a new proposal for the next meeting.

Outstanding project proposals from previous meetings.

**Design and synthesis of well-defined polymeric structures**
Proposer: Puskas

Aim: Produce and characterise (in particular rheology) of model PIB and PS polymers having various branching structures. UWO to produce the model systems (stars, arborescent, pom-pom, 0.5kg batches).

Status: Puskas to circulate a draft proposal (with input from Gunesin and Dijkstra)

A link to commercial systems is needed to give relevance to this working party.

**Polymer composites of different aspect ratios.**
Proposer: Goeschel.

Although a new proposal was available from Goeschel, the scope of the project was still not clear. Bailey will recontact Goeschel and work this up into a project proposal for presentation at the Paris meeting.

Bucknall asked if C fibres would be of interest. BASF may be willing to provide materials.

**Old title: Critical Morphology parameters in composites.**
Goeschel is still interested in starting a project on composites. At Ludwigshafen he presented a brief summary of fibre length and fibre orientation in which the short fibre and long fibre systems with curved fibres were considered. In Karlsruhe Goeschel presented a similar proposal, and it was agreed that a tactical plan would be formulated. Goeschel is l/d ratio from 1 to greater than 100. In nano-tube we have an aspect ratio of 300. Prediction of mechanical properties is also possible. Bailey can help with a tactical plan.

**Thermodynamics and structure of water soluble polymers and blends**
Proposer: Schubert.

Schubert was not present.

Aim: Correlation between thermodynamics and chemical structure of commercial (bulk) materials. Example: correlate intrinsic viscosity, spin coating film thickness and molecular weight. To be used as characterisation or predictive tool or as preparation of well defined substrates. Effect on biodegradability.

Status: Schubert to select materials and to circulate draft proposal.

Update – still pending.

**High resolution GPC for linear and branched polymers.**
Proposer: Puskas

This project will be defined in 2004 by Puskas. A proposal will be put together for the Paris meeting.
Aim: Use technique (UWO developed multi-column GPC) for elastomers and possibly plastics and correlate with linear viscoelastic rheology and mechanical properties to get molecular information on polymers that are quite similar in standard characterisation methods.
Status: Proposed as possible add-on to a study which deals with similar polymers. Use PE as a starting material. Look at LDPE samples from FEM simulation. Link with 'well defined polymeric structures' project.

Flow properties of processing of uncrosslinked elastomers.
Proposer: Kaszas

Kaszas reminded the group the aim of this project. Bayer will decide either to cancel the project or to work up the project for the Paris meeting.

Aim: Apply polymer rheology techniques (simple shear rheometry, capillary rheometry including extrudate properties, Rheotens test) to elastomers of e.g. PDMS, butyl rubber (different Mooney viscosities), or high MW PIB.

Check the applicability of rheometry (more or less standard for polymer melts) for rubber materials, for shear stress, first normal stress difference, capillary rheometry and rheotens.
Proposer: Kaszas.

Rheometrics molecular weight distribution calculation software now available – is it valid? Is the Rheotens valid for rubber characterisation? A proper rubber sample would be chosen (e.g EPDM and Butyl rubber as 2 starting system). Later apply to ethylene/polypropylene copolymers. Pure elastomers would be used with calcium stearate as an anti-coagulant.

Nanocomposites
Proposer: Lyngaae-Jorgensen.

Characterisation of polymer containing these systems – is there some commercial material available? Toyota produce this, also Bayer PA12, Basell in US have some speculative interests. The proposal may be premature at this stage. Dijkstra suggests that only characterising the Bayer material would be problematic. Also processing these systems would very helpful. Bucknall suggest that the techniques used for characterising these materials would be prudent. The EA Group are also looking into this as a feasibility study, with 2 material suppliers. This should be further discussed.

Measurement of Die Swell (esp. PE)
Proposer: Ourieva

Die Swell and on-line behaviour and property performance need to be related. Laun said there is not a unified approach. This needs better definition – perhaps limit to a annular die. (closer to blow moulding). Meissner said we should refer to it as extrudate swell. Computation simulation may also be included for predictive techniques. A literature review is needed first because a lot of work has been done, and then a plan made. Advances in extensional flow and in constitutive equations and moved the subject on, and this should be consolidated before agreeing a proposal.
In industry a common platform for a technique that is in everyday use would be useful. Laun thought this might follow the Future recommendations in the characterisation of continuous fibre composites example, in that this is a non-experimental study.
Extrusion coating linked to rheology
Proposer: Ourieva

Zoetelief had contacted Ouvrieva and the project needs to be redefined.
Identifying the comparison between labs and improve quality of measurements. The validity of measurements and models to the extrusion coating process will be assessed. Ourieva will come back to the WP having explored the possibilities. Zoetelief is also interested to define the scope.

Techniques to study commercial nano-composites using organic clays.
There is now a new project on this through Kim and this will be incorporated into the EA project.
Proposer: Lyngaae Jorgensen.

The proposer would like Utracki to be involved in this. Processing behaviour will be included. Melt rheology and structural characterisation – Goeschel would be interested in contribution for TEM and X-ray measurements.

PHB Biopolymers could be studied
Proposer: Koopmans.
Rheological and structural characterisation of biodegradable polymers should be studied and advanced in general. A more formal project proposal was planned for the Scotland meeting, but will now be made in Paris hopefully.

Critical assessment of rheological measurement equipment
Proposer: Max Ruellmann
Ruellmans showed examples of erroneous data from friction or drift in air bearings. Another case showed that the temperature control gave the wrong slope for zero shear viscosity and f(Mw). Gap height dependence of G’ arises from inertial effects in the fluid (apparent G’ values for a purely viscous fluid can be predicted).
Limits and critical points need to be identified, with reference materials, similar problems and share and report this together. Exchanging ‘tricks’ and pulling this together is proposed. Ruellmans will circulate a document and tactical plan and to ask for participation before the Paris meeting.

Creep interpolation techniques – to obtain accelerated data generation.
Proposer: Ian Robinson,

NPL will be visited and a literature review will be carried out on linear viscoelastic t-T superposition. Kaszas is interested in extending this work to elastomers. Bayer would also be interested in providing materials. Robinson or Bailey will present a proposal in Paris.
Tailor-Made Chitosan For Sustained Release of Drugs Studies.
Proposer: Mohammad M. Fares
(this proposal has been sent by Prof. Fares for our consideration. He is from the Dept. of Applied Chemistry, Jordan University of Science & Technology, and aims to start the project (if we can agree to participate) at the Paris meeting. Please contact him to offer support for the project at his e-mail address: fares@just.edu.jo)

INTRODUCTION
Chitosan is a derivative of chitin that is extracted from crustaceans such as crab, shrimp and cuttlefish. It is finding lots of interest due to excellent properties such as biodegradability, biocompatibility, non-toxicity, adsorption and pharmaceutical applications. The much-explored area for the graft copolymerization is reported mainly using chemical routes.

Grafting of chitosan with various vinyl monomers was done using different initiators such as n-butyl lithium, epichlorohydrine, sodium alginate, and ceric ammonium nitrate (CAN). Grafting of natural polymers using CAN has been finding lots of interest due to simple mechanism electron transfer, low activation energy and formation of free radicals on Chitosan. The hydrogel formation is gaining large scale of interest in controlled release bioactive materials and used as carriers for delivery of various drugs.

Aims & Goals of the project:
Our present studies aims at preparation and characterization of Freeze dried and air dried chitosan-g-PolyA semi-interpenetrating networks (semi-IPN), where A can be acrylate and acrylic acid derivatives. The aim of these different derivatives is to create a site-specific drug delivery, in the oral cavity, stomach, small and large intestine using novel formulation designs.

Different antibacterial and antibiotics can be used like Sulphadiazine, Amoxicillin, Metronizazole, Diclofenac sodium, and others will be incorporated in the microspheres and the in vitro (and if possible in vivo studies) release profiles will be established both in simulated gastric and intestinal fluids.

Methodology
The proposed procedure would be focused in three stages:
- Preparation and optimization the different conditions of chitosan-g-PolyA, such as optimization of Monomer conc., Initiator conc., polymerization Temperature, polymerization Time, and Material to Liquor ratio will be tracked and followed up in terms of %grafting efficiency (%GE).
- Formation and optimization of novel semi-interpenetrating network (semi IPN) using N, N'-Methylenebisacrylamide crosslinker to create different porous systems that are able to maintain different sizes of antibiotic molecules in cavities.
  In vitro release profiles will be established both in simulated gastric and intestinal fluids for the different formulations using different porous sizes and the optimum values will considerably be determined.

Characterization
The characterization of the grafted chitosan will be done using FTIR, NMR, and X-ray. Thermal analysis will further assist in interpreting the data like TGA and DSC. Furthermore, SEM will be used in morphology studies.
  In vitro release profile will be established at pH 1.2 and 7.4 at 37 °C. Aliquots will be taken at regular intervals and assayed spectrophotometrically and particle size analyzer will be used for porosity studies.