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The objective of the research in this subprogram is to develop software and constitutive models for the prediction of the final properties of polymer articles, and the dependence of these properties on the processing history.

The quality of a manufactured polymer product depends on the nature of the processing, the processing history and the properties of the polymeric material. Currently, commercially available injection moulding software allows rational and optimal design of the moulds but cannot reliably predict the mechanical properties of the injection moulded parts. These limitations can be overcome by refinements that incorporate the results from systematic research on polymer properties and rheology. The projects in this subprogram will investigate improved constitutive models for process simulation, the development of microstructure during processing, and the dependence of final properties on this microstructure.

THE PROPERTIES OF INJECTION MOULDED PARTS: PREDICTION FROM MOULDING CONDITIONS

OBJECTIVE

To develop software that can predict the properties of injection moulded plastic components.

BACKGROUND

Injection moulding processors can use commercially available software for process models and optimal mould and part design; however, the limitation of this software is that it cannot predict the properties of parts or their dependence on the moulding and solidification conditions.

The general aim of the project is to improve the accuracy of modelling the complete mechanical/ thermal/geometrical behaviour of polymers as they cool from the melt to the finished product during the

From left: Project team members Dr Peng Zhu and Associate Professor Graham Edward from Monash and Dr Guangwei Liu (CRC-P)

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injection moulding process. The project is examining the overall injection moulding process by dividing it into two stages:

- *The processing history and how it determines the molecular arrangement in the solid moulding and the molecular morphology.* The processing history can be predicted using the existing Moldflow software, but some aspects of this will require further refinement.
- *The dependence of the final properties of a moulding on the distribution of the morphology throughout the moulded article.* This will involve the production of moulded parts under carefully controlled conditions, the microstructural characterisation of these specimens and the evaluation of their properties. The modelling of the effects of the heterogenous microstructure found in mouldings will be a key aspect of this stage of the project.

PROGRESS AND ACHIEVEMENTS

The research has continued the characterisation of the molecular morphology of polypropylene injection mouldings using polarised light optical microscopy of microtomed thin sections, X-ray diffraction and thermal techniques. Analysis of the extensive X-ray diffraction results for a range of samples, using the high-intensity synchrotron source at the Photon Factory in Tsukuba, Japan, is nearing completion. In particular, samples moulded under a range of controlled conditions have been characterised using wide-angle X-ray scattering and small angle X-ray scattering. This information is providing extremely valuable insights into the factors influencing the final mechanical properties of the moulded sample.

"Modelling of mechanical properties has continued, and linking these microstructures to thermomechanical histories is proceeding."

Mechanical measurements on a number of polypropylene injection mouldings have also been performed, quantifying the expected anisotropy of the material and relating this back to the physical properties of the sample. Modelling of mechanical properties has continued, and linking these microstructures to thermomechanical histories is proceeding. In order to further progress the modelling studies, research on the properties of materials with idealised microstructures has commenced.

PROGRESS AGAINST MILESTONES	
Simulate moulding trials to correlate stress/temperature histories with morphologies.	Achieved
Commence research on developing 'model materials' and relate microstructures with mechanical properties.	Achieved
Develop numerical methods to predict the mechanical properties of injection-moulded samples.	Partially achieved

CONSTITUTIVE MODELLING FOR POLYMER PROCESSING

OBJECTIVE

To improve the accuracy of modelling the complete mechanical/thermal/geometrical behaviour of polymers as they cool from melt to finished product during the injection moulding process.

BACKGROUND

Polymer processing typically involves melting and solidification of the material, and development of process-induced molecular orientation and crystalline structure. Currently no model can describe this range of behaviour.

The project aims to develop a viscoelastic constitutive model that can be used for realistic modelling of polymer processing. The main features of the proposed model are: quantitative accuracy in representing the rheological response, compressibility, effect of crystallisation, and liquid-solid phase change; predictive capability for frozen-in stresses, birefringence and molecular orientation; computational tractability and simplicity; and the ability to experimentally determine the parameters involved in the constitutive equation.

To be relevant to industry, data for the model must be obtained, making the property measurement an integral part of the project. The model, to be used as an industry standard, will be incorporated into existing software packages, refined through trials by participants that are processors, and commercialised by Moldflow.

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Some members of the Constitutive modelling for polymer processing team: (from left) Dr Matti Keentok (USYD), Mr Vangu Kitoko (CRC-P student), Professor Roger Tanner (USYD), Dr Howard See (USYD), Dr Gerald Pereira (USYD) and Dr Simin Nasseri (USYD)

PROGRESS AND ACHIEVEMENTS

Research on the crystallisation of polymers under shear has continued, with some theoretical advances made on the interaction of stress, crystallisation and rheology. In particular, the behaviour of LDPE and polypropylene after a sequence of mechanical and thermal histories in simple flows has been measured. The replication of some interesting results on polypropylene crystallisation under shear has been achieved.

> "Implementation of the research outcomes… in the Moldflow code has begun…"

Implementation of the research outcomes flowing from this project, and the research on *The properties of injection moulded parts: prediction from moulding conditions,* in the Moldflow code has begun, with several concepts being trialled in development coding. The correlation between experimental results and Moldflow simulation appears to be promising, with the Moldflow software having been modified to take account of the effects of shear on crystallisation.

PROGRESS AGAINST MILESTONES	
Develop quantitative methods for characterising polymer morphology and orientation.	Achieved
Examine the behaviour of LDPE and PP under shear conditions and determine the impact on the crystalline properties.	Achieved
Start including the results of the research in the Moldflow code.	Achieved

SUBPROGRAM RESEARCH PLANS FOR 2001/2002

The properties of injection moulded parts: prediction from moulding conditions. Research on the crystalline morphology mapping, and particularly the correlation with simulations, will continue. An improved understanding of the modelling of crystalline and amorphous polymers will be developed.

Constitutive modelling for polymer processing. Numerical modelling of shear-induced crystallisation involved in the injection moulding process will continue. The examination of the solidification of polymers under shear will also be pursued and the models further developed.