Australian-Korean Rheology Conference 2001

Program

Wednesday 19th September 7:30 PM Reception

Thursday 20th September

09:00 AM

Plenary Lecture

Theoretical explanation of process stability enhancement by the encapsulation extrusion coating method

- Professor Jae Chun Hyun

	Session 1	Session 2
	Suspensions and Emulsions	Polymer solutions, surfactants and gels
09:40 AM	Magneto-rheological suspensions: Relationship between microstructure and rheological response - Dr Howard See	Large amplitude oscillatory shear experiment as a way to probe the microstructure of a complex fluid system - Professor Kyung Hyun Ahn
10:00 AM	Rheological study of eutectic mixture of alkali sulphates and silica as a model of coal ash at high temperatures - Mr N Tonmukayakul	Numerical and experimental investigations into the deformation of drops in complex flows - Dr Justin Cooper-White
10:20 AM	Morning Tea	
10:40 AM	A Newly Proposed Scaling Equation of Yield Stress for Electrorheological Fluids - Professor Hyoung J. Choi	A New Technology for the Investigation of Low-Vis cous Structural Fluids - Dr Seungrok Kim
11:00 AM	Shear Thickening in a Coarse Nickel Sulphide Tailings Slurry - Mr Andrew Chryss	A model for the viscoelastic behaviour at gelation based on the relaxation behaviour of branched molecules - Ms Nara Altmann
11:20 AM	The Effect of Temperature on the Yield Stress of Mineral Suspensions - Dr Ross de Kretser	Flow induced microstructure transitions of wormlike micellar solutions with water-soluble polymer - Dr Won-Jong Kim
11:40 AM	Use of the vane in steady shear to minimise slip in high yield stress suspensions and emulsions - Dr George Franks	Alignment and aggregation of spherical particles in viscoelastic fluid under shear flow - Professor Chongyoup Kim

12:00 Lunch

01:40 PM

Plenary Lecture

Simulation for behavior of aggregated colloids in flows and the application to the suspension rheology

- Professor Ko Higashitani

	Polymer melts and liquid crystalline systems	Numerical Methods
02:20 PM	Rheological Properties and Phase Inversion of Polypropylene; Poly(styrene-co-acrylonitrile) Blends - Professor Woo Nyon Kim	Rheometrically resolvable flows at Intermediate Reynolds numbers: hours of fun with the unsteady Stokes equation - Dr Adam Burbidge
02:40 PM	Predicted Rheological Properties of Liquid Crystalline Polyesters by Molecular Simulation - Mr Dumitru Pavel	Numerical simulation of the mold filling in foam reaction injection molding - Mr Dongjin Seo
03:00 PM	Direct analysis of entanglements in the atomic structure of high polymer melts - Dr Alfred Uhlherr	Mathematical characteristics of the pom-pom model - Professor Youngdon Kwon
03:20 PM	Afternoon Tea	

Rheological and mechanical properties of syndiotactic polystyrene/organoclay nanocomposites

- Mr Won Mook Choi

Modeling of reaction injection molding process of phenol-formaldehyde resin filled with wood dust

- Mr Jae Wook Lee

Preparation of Metal Film by Spin Coating Method

- Mr Hak-Ju Kim

Study of the variation of rheological properties in the process of colloidal silica coatings prepared by sol-gel method

- Mr Hvun Uk Kang

Large amplitude oscillatory shear behavior of polymer solutions: poly(vinyl alcohol), xanthan gum, hyaluronic acid

- Mr Kyu Hyun

Scale up of viscosity measurement of concentrated suspensions from conventional rheometer to stirred tank reactor

- Mr Ange Nzihou

Synthesis of Thermoplastic Nanocomposites by Two-Stage Sonication Process

- Mr Pil Soo Lee

Rheological and thermal properties of long chain branched polypropylene.

- Mr J.H. Yoo

Effect of fluid viscoelasticity on the draw resonance dynamics of film casting process

- Mr Joo Sung Lee

Dense fly ash - water slurry transportation with additive feeding system for restarting of pipeline

- Mr Lei Li

Yield stress measurements of titanium dioxide particle suspensions

- Mr Masanari Ishizuki

Numerical simulation of viscoelastic flow in expansion/contraction channel.

- Ms L. Saoudi

Rheological Properties of Poly(vinyl alcohol)/Hyaluronic acid blends

- Ms Sook Hyun Kim

The rheology of bread dough made from four commercial flours

- Mr Matti Keentok

Comparison of Cylinder and Cone Geometries for Yield Stress Measurement with the Slump Test

- Mr Sam Clayton

The Plasticisation Effect of Glycerol on The Gelatinisation of Wheat Starch

- Ms Gena Nashed

Flow and Additive effects on the mesoporous silica structure fabricated by using block copolymer templates

- Mr Dae-Geun Choi

Applications of rheology in suspension dewatering

- Mr Shane Usher

Determination of the discrete relaxation spectrum from dynamic moduli using a nonlinear regression method

- Dr G. Sodeifian

Ternary Blended Polyethylene Films: A Study on its Mechanical and Thermal Properties.

- Rahul Kumar Gupta

Synthesis of Polyaniline-surface modified clay composites for application of electrorheological fluids

- Mr Jong Hyeok Park

Conference Dinner

Thursday 07:00 PM

Gadsden Hall, Melbourne Business School

Friday 21st September

09:00 AM

Plenary Lecture

Transportation of ice slurry to reduce the pumping power for energy saving cooling system

- Professor Hiromoto Usui

	Session 1	Session 2
	Polymer processing	Polymer solutions, surfactants and gels
09:40 AM	A Novel Method to Measure the Melt Viscosity: the Screw Rheometer - Dr Shi-Ho Lee	An overview on the swirling flow of non-Newtonian fluids - Dr Jason Stokes
10:00 AM	Melting Phenomena and mechanism in polymer processing equipment - Dr Myung-Ho Kim	Effect of degree of saponification on the rheological properties of syndiotactic poly(vinyl alcohol)/water solution - Professor Bong Shik Kim
10:20 AM	Morning Tea	
	Polymer melts and liquid crystalline systems	Numerical methods
10:40 AM	Polyethylene flow prediction with a differential multi- mode Pom-Pom model - Dr R.P.G. Rutgers	Numerical Investigation of Interface Deformation in Stratified Coextrusion Flow of Viscoelastic Fluids - Professor Seong Jae Lee
11:00 AM	Effect of Macromolecular properties on shear rheology of low-density polyethylene (LDPE) - Dr Rahul Gupta	Extracting the memory and relaxation functions of viscoelastic fluids from small amplitude oscillatory shear data - Dr Leong Yeow
11:20 AM	Estimation of polydispersity index of branched polypropylene by rheological techniques - Mr Debashis Roy	Gaussian Approximation for Hookean Dumbbells with Hydrodynamic Interaction and Excluded Volume - Dr J Ravi Prakash
11:40 AM	Rheological and mechanical properties of ABS/PC blends - Dr Masud Khan	

12:00 Lunch

01:40 PM

Plenary Lecture

Numerical Simulation of High Weissenberg Number Problem in a 4:1 Planar Contraction Flow

- Professor Seung Jong Lee

	Polymer processing	Polymer solutions, surfactants and gels
02:20 PM	Measurements of fluid model parameters of PET for stretch blow molding simulation - Dr Hern-Jin Park	Macromolecular Dynamics in Shear at Concentrations above Critical Overlap Dr David Dunstan
02:40 PM	The influence of die geometry and extrusion rate on the melt strength meaurment of polypropylene - Dr Andro Lau	The measurement of viscosity in a gelling suspension - Dr A.F. Collings
03:00 PM		Instabilities and other problems in parallel plate rheometry - Dr M. Keentok
03:20 PM	Afternoon Tea	
	Suspensions and Emulsions	
03:40 PM	Rheological Characterisation of Rapid Settling Slurries - Mr Timothy Akroyd	Structure for hydrophobically modified hydroxy-ethyl cellulose in the presence of an anionic surfactant - Dr Viyada Tirtaatmadja
04:00 PM	Compressional Rheology of Suspensions - Prof. Peter Scales	Effects of rotating speed on the patterns of particle segregation in a rimming flow of polymer solution - Professor Do Hyun Kim
04:20 PM		Calibration of a commercial instrumented measuring kneader for rheological applications - Dr T. Kealy

04:40 PM

Close of Conference

Theoretical explanation of process stability enhancement by the encapsulation extrusion coating method

Jae Chun Hyun and Joo Sung Lee

Department of Chemical Engineering, Korea University, Seoul 136-701, Korea

jchyun@grtrkr.korea.ac.kr

A film casting simulation has been used to demonstrate why the encapsulation extrusion coating process is so effective industrially in enhancing the stability of the extrusion coating of low-melt-strength polymers like HDPE. In the present study, it is intended to explain theoretically why and how the co-extrusion of high-melt-strength polymers like LDPE in encapsulation dies improves the HDPE process. The undesirable neck-in and draw resonance phenomena frequently occurring in the extrusion coating of HDPE are shown due to its extension-thinning viscosity property, and consequently can be alleviated using extension-thickening viscosity materials like LDPE in the encapsulating dies.

Keywords: encapsulation, extrusion coating, stability analysis

Magneto-rheological suspensions: Relationship between microstructure and rheological response Howard See and Roger Tanner

School of Aerospace, Mechanical & Mechatronic Engineering, The University of Sydney, Sydney 2006, Australia howards@mech.eng.usyd.edu.au

A magneto-rheological suspension consists of magnetisable particles dispersed in a non-magnetisable carrier fluid, and displays a dramatic increase in viscosity under a magnetic field. The basic mechanism is that the field induces polarisation in each particle, and the resulting interaction forces lead to the formation of elongated aggregates which increase the viscosity. Our understanding of the relationship between the mechanical response and the aggregate microstructure is still incomplete. This work probes the characteristics of the aggregates under strong magnetic fields through a series of rheological measurements, including oscillatory shearing, oscillatory deformations superposed on steady shear flow, and very low shear rate tests. The results are interpreted within the framework of the dipole-dipole interaction model.

Large amplitude oscillatory shear experiment as a way to probe the microstructure of a complex fluid system

Kyung Hyun Ahn, Seung Ha Kim, Hoon Goo Shim and Seoung Jong Lee

School of Chemical Engineering, Seoul National University, Seoul 151-744, Korea ahnnet@snu.ac.kr

In this talk, we suggest a possibility of LAOS (Large Amplitude Oscillatory Shear) experiment as a way to probe the microstructure of a complex fluid system. We will classify the complex fluids depending on the behavior of rheological properties under

LAOS experiment. Their complex behavior will also be investigated in terms of higher harmonic contributions in the shear stress response by using the Fast Fourier Transform (FFT) method. We will explain their complex behaviors in terms of the molecular parameters of a network model.

Keywords: LAOS (large amplitude oscillatory shear), complex fluid, FFT (fast Fourier transform), network model

Rheological study of eutectic mixtures of alkali sulphates and silica as a model of coal ash at high temperatures

N Tonmukayakul¹ and Q D Nguyen²

¹Cooperative Research Centre for Clean Power from Lignite ²Department of Chemical Engineering, The University of Adelaide, Adelaide 5005

Australianarong@chemeng.adelaide.edu.au

In fluidised-bed combustion and gasification of low-rank coal, the chemical composition and transformation of the inorganic matter in the coal ash may contribute to operating problems such as agglomeration and defluidization. It has been found that the key constituents in coal responsible for ash deposition, which potentially leads to agglomeration are alkali sulphates, mainly of sodium, calcium and magnesium. The combinations of these constituents easily form low melting point eutectics, which melt and bind bed particles into agglomerates at temperatures well below the operating temperature. Thus, in order to understand the mechanisms involved in ash deposition and agglomeration, it is fundamentally important that the rheological behaviour of mixtures of these key constituents be studied as a function of their compositions and operating temperature. Using a recently developed high temperature rheometer, the rheological properties of synthetic eutectic mixtures containing Na2SO4, CaSO4 and MgSO4 at different proportions have been measured. The data obtained have been used to develop a statistical model that can satisfactorily describe the rheological properties as a function of chemical compositions of several Australian brown coal and lignite. In recent work, we have found that inclusion of the presence of unmelted solid phase, eg. silica, in the study of the rheological behaviour of the molten alkali sulphate can significantly improve the model for accurately predicting the rheological characteristics of low-rank coal ash at different temperature and processing conditions.

Keywords: high-temperature rheology, coal ash rheology, alkali sulphate cutectic, rheological characterisation

Numerical and Experimental Investigations Into the Deformation of Drops in Complex Flows Justin Cooper-White, David Whyte, Malcolm Davidson and David Boger

Particulate Fluids Processing Centre Department of Chemical Engineering, The University of MelbourneVictoria 3010, Australia jjcw@unimelb.edu.au

The production of oil-water emulsions of predetermined droplet

sizes are paramount to the successful market acceptance of many products within the food, cosmetic, pharmaceutical and photographic industries. An understanding of the deformation history and breakage of one liquid drop within another liquid is thus of vital importance. Contraction flows can deform drops by increasing the velocity gradients experienced by a drop and as a result, are a principle design feature of many industrial emulsification operations. For example, a high pressure homogeniser, consisting of a pipe constricted by an orifice plate, is often used to break drops of oil dispersed in an aqueous based continuous phase. This paper explores experimentally and theoretically the transient deformation of a single drop in a contraction flow. Effects such as contraction geometry, initial drop size and continuous phase solution characteristics are explored. Preliminary results of the numerical simulations used to predict the drop motion and its deformation, based on finite difference and volume-of-fluid numerical techniques, are provided and compared with the observed shapes from experiments.

A Newly Proposed Scaling Equation of Yield Stress for Electrorheological Fluids Hyoung J. Choi, Ji W. Kim and Yun H. Cho

Department of Polymer Science and Engineering, Inha University,Inchon 402-751, Korea hjchoi@inha.ac.kr

The electrorheological (ER) fluids exhibit a dramatic change in rheological and electrical properties, and among these properties a yield stress is known to be the most important characteristic for adapting the ER fluids to the application device. In this study, we present a universal curve representative of the yield stress dependence on electric field strength for ER fluids. The newly proposed scaling equation incorporates both the polarization and conductivity models. Yield stress data for various ER fluids are collapsed into a single curve for a broad range electric field strengths, suggesting that the scaling equation we proposed is adequate for predicting the ER property.

Keywords: electrorheological (ER) fluid, yield stress scaling

A New Technology for the Investigation of Low-Viscous Structural Fluids Seungrok Kim

Thermo Haake Regional Office Seoul 140-210, Korea kim.seungrok@thermohaake.com

Fluids of higher viscosity dampen inertial effects more than samples of lower viscosity. Additionally, inertial effects become greater as frequency increases. This leads to the fact that, for low-viscous structural fluids such as polymer solutions, emulsions or colloidal dispersions, there is some maximum frequency at which inertial effects can no longer be corrected. Many so-called universal rheometers with conventional set-ups turned out to have this inertial limit during dynamic testing for such samples. An innovative solution for the measurements on low-viscous structural fluids is presented. The performance of

the new technology is demonstrated and several test results are presented.

Keywords: inertia limit, viscoleasticity, dynamic oscillatory measurements

Shear Thickening in a Coarse Nickel Sulphide Tailings Slurry

Andrew Chryss¹, Sati Bhattacharya¹ and Lionel Pullum²

¹Rheology and Materials Processing Centre, RMIT University, Melbourne 3000, Australia andrew.chryss@rmit.edu.au

The increased use of thickened tailings discharges and co-disposal with coarse material has created many examples of slurries with complex rheological behaviour. One such example is a tropical nickel sulphide tailings. This slurry displays shear thickening behaviour above a critical shear rate combined with thixotropy. Both these phenomena occur in the shear rate range of processing interest but require specialised testing methods to separate their contribution to the slurry rheology. The shear thickening effect is partly due to the presence of mineral fibres but an additional mechanism is indicated as critical shear rate for onset changes with overall volume fraction and polydispersity, as do the parameters in the constitutive equation.

Keywords: shear thickening, tailings, slurry rheology

A model for the viscoelastic behaviour at gelation based on the relaxation behaviour of branched molecules

Nara Altmann and Peter J Halley

Department of Chemical Engineering, The University of Queensland, Brisbane 4072, Australia naraa@cheque.uq.edu.au

Chemical gelation is characterised by a power law distribution of molecular weight and self-similarity of the network structure. These characteristics determine a particular rheological response at the gel point. Previously a number of investigations have focused on understanding the viscoelastic behaviour at the sol-gel transition. These models however, assume a fractal dimension distribution of the relaxation modes, thus obtaining the power law behaviour at gelation. In this work we are able to predict the power law behaviour of the relaxation spectrum based on a relaxation pattern adapted from the group interaction model [1] for linear and branched polymer molecules. Our results show that the power law behaviour occurs due to a combination of the relaxation of short and long branches of the network chain and relaxation of the molecules in the sol fraction. The distribution of molecular weights and branch architecture of the network chain is obtained through a Dynamic Percolation Grid Monte Carlo Simulation. The model results are compared with the experimental data for an epoxy-amine thermoset system.

 D Porter, Group Interaction Modelling of Polymer Properties, Marcel Dekker, NY, 1995.

Keywords: gelation, viscoelastic model, branched polymers

The Effect of Temperature on the Yield Stress of Mineral Suspensions

Ross de Kretser and Peter Scales

Particulate Fluids Processing Centre
Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia
rgdk@unimelb.edu.au

The yield stress of suspensions is commonly believed to decrease with increasing temperature. To probe this belief, tests were conducted on suspensions of Zirconia over a range of inter-particle force conditions and temperatures. Measurements showed that the yield stress of zirconia increased by up to 50% between 15 and 45 deg C. Using inter-particle force considerations, the temperature dependence of the yield stress was modelled. Model predictions agreed with the results for temperature changes from 15 to 25 deg C, however above 25 deg C, yield stresses were underpredicted. Potential reasons for the discrepancy will be discussed. *Keywords*: yield stress, temperature dependence, modelling

Flow induced microstructure transitions of wormlike micellar solutions with water-soluble polymer Won-Jong Kim, Justin Cooper-White and David Boger

Particulate Fluids Processing Centre
Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia
wk@unimelb.edu.au

We present a novel approach to isolate the flow-induced microstructure transition of wormlike micellar solution simply plotting by shear viscosity versus the shear stress. This allows the critical stress to be definitely defined. We discuss the solid-to-liquid transition of CTAB/NaSal micellar systems, which related to the disruption of the long range/short range interactions. In addition, we investigate the effect of hydrophobicity in polymer on this structure transition as dependent on the surfactant concentration.

Keywords: wormlike micelle, transient yield stress, water soluble polymer

Use of the vane in steady shear to minimise slip in high yield stress suspensions and emulsions George V.Franks

Department of Chemical Engineering, The University of New-castle, Callaghan 2308, Australia cggvf@cc.newcastle.edu.au

Results are presented which indicate that the use of a vane tool in steady state shear measurements provide improved rheological data compared to the solid Couette. The solid bob tends to slip at the suspension or emulsion interface when the yield stress of the fluid is high. The use of a vane minimises the possibility of slip at the suspension tool interface, both solid bob and vane geometries were compared with an industrial minerals tailing and a concentrated water in oil emulsion.

Keywords: vane, suspension, emulsion

Alignment and aggregation of spherical particles in viscoelastic fluid under shear flow

Chongyoup Kim and Daejin Won

Department of Chemical Engineering, Korea University, Seoul 136-701, Korea cykim@grtrkr.korea.ac.kr

Rheology and microstructure of filled polymeric liquid are of great importance both practically and academically. In this study, we performed a series of experiments on the migration of spherical particles suspended in viscoelastic liquid and investigated the chaining and aggregation of particles under simple shear or torsional flows. The result shows the chaining and aggregation are strongly affected by the shear thinning effect in addition to the normal stress difference. The mechanism of particle chaining will be discussed in the presentation.

Keywords: elasticity, shear thinning, aggregation mechanism

Simulation for behavior of aggregated colloids in flows and the application to the suspension rheology

Ko Higashitani and Kenji Iimura

Department of Chemical Engineering, Kyoto University, Kyoto 606-8501, Japan

higa@cheme.kyoto-u.ac.jp

A three-dimensional modified discrete element method in which the "effective" hydrodynamic drag force and the disturbance of neighboring particles on the flow field are taken into account is proposed to simulate the deformation and breakup process of large arbitrary aggregates in flows. First, the dynamic shape factor of rectangular aggregates is simulated and compared with the corresponding experiment, showing that the method can predict the behavior of aggregates in fluids quantitatively. Secondly the method is applied to simulate the breakup of large aggregates in shear and elongational flows. It is found in simple shear flows that the average number of particles in broken fragments is given by a universal function of NDA (the ratio of the representative hydrodynamic drag force and the adhesive force), independently of various conditions, and that the results agree well with experiments reported elsewhere. Finally it is shown that the proposed model is applicable to evaluate rheological properties of suspensions composed of unstable coagulated particles.

Keywords: unstable aggregates, suspension rheology, DEM simulation

Rheological Properties and Phase Inversion of Polypropylene-Poly(styrene-co-acrylonitrile) Blends W.N. Kim, H S Paik, J H Park and M S Han

Department of Chemical Engineering, Korea University, Seoul 136-701, Korea kimwn@korea.ac.kr

Phase inversion of the polypropylene (PP)/poly (styrene-co-acrylonitrile) (SAN) blends has been investigated by Advanced

Rheometric Expansion System (ARES), capillary rheometer, extension rheometer, and scanning electron microscopy (SEM). Values of the shear and extension viscosity ratio were used in the Utracki, the Miles and Zurek, and the Metelkin and Blekht models to obtain the weight fraction of phase inversion for the blends. For the Utracki model, the weight fraction of phase inversion for the PP in the PP/SAN blend was found to be 0.32 and 0.41 for the shear viscosity ratio and extension viscosity ratio, respectively. From the results obtained by morphological studies, the phase inversion was found in the region of 45/55 PP/SAN blends. The phase inversion for the PP in the PP/SAN blends is compared between the several models obtained by rheological measurements.

Keywords: polymer blends, phase inversion, extension viscosity

Rheometrically resolvable flows at Intermediate Reynolds numbers: hours of fun with the unsteady Stokes equation

Stokes equation Adam S. Burbidge^{1,2}, Colin Servais¹ and Alexandre I. Romoscanu^{1,3}

¹Nestlé Research Center, Lausanne 26, Switzerland adam. burbidge@rdls.nestle.com

²School of Chemical Engineering, University of Birmingham, Edgbaston B15 2TT, UK

³Institute of Mechanical Systems, ETH Zurich, Zurich, Switzerland

Traditionally, rheometric measurements are made under the assumption of a vanishingly small Reynolds number which admits solutions of a pseudo-static force equilibrium equation i.e. the divergence of the stress tensor is zero. In the case of simple shear flows, this steady Stokes equation reduces to a second order ODE for generalised Newtonian fluids, which can be easily solved. However, for viscoelastic materials, there is natural time dependency due to the material memory, which induces a phase shift. Unfortunately, if the vanishingly small Reynolds number assumption is relaxed, then there is an inherent time dependency in the force balance equation since the time dependent inertial term can be balanced by the divergence of the stress tensor. The consequence of this is that any experimentally measured phase shift is a convolution of material and inertial effects. In many practical cases (particularly when we wish to obtain the material relaxation time spectrum) we are interested in measuring material response functions under high frequencies and shear rates, so it would be useful to be able to remove inertial effects from experimental measurements. In principle, at least, this can be achieved by solving the unsteady Stokes equation instead of the more usual steady Stokes equations. In this paper we examine the possibility of deconvoluting inertial and material effects for non-vanishing Reynolds number flows. We also discuss the consequences for multiwave oscillation and general Fourier analysis of response signals, and comment on the onset of fluid dynamical flow instabilities.

Predicted Rheological Properties of Liquid Crys-

talline Polyesters by Molecular Simulation Dumitru Payel, Irina Yarovsky and Robert Shanks

Department of Applied Physics, RMIT University, Melbourne 3000, Australia

dumitru.pavel@rmit.edu.au

Computer simulation have been proved as an important research tool for simulating structures and predicting physical, chemical, rheological and liquid crystalline properties of polymers in our previous studies. Molecular simulation can be considered as a bridge between experimental and theoretical study. The simulation study is a challenge for the future research and can bring much faster new polymers and materials on the market. Also the cost of molecular simulation study is much lower then experimental one. Experiments cannot be performed on materials that have not yet been developed. For this research we applied molecular simulation techniques, such as molecular mechanics and molecular dynamics to simulate chemical structures and predict the rheological properties of thermotropic main-chain liquid crystalline aromatic polyesters. The motivation behind this study is determined by the wide range of applications of liquid crystalline polymers in industry and their unique properties. They exhibit long rage orientational order. The properties of thermotropic liquid crystalline polymers are governed by temperature changes. Computations and conformational analyses were carried out using molecular simulation software for material science, Cerius2 version 4.0, designed by Molecular Simulations Incorporated, San Diego, USA. Single chains and unit cells of the polymers with degree of polymerisation equal to 15 have been used for these molecular simulation studies. The initial macromolecular conformations of the simulated polymers were optimised and the value of the total potential energy and its components of the investigated polymers were obtained.

Keywords: rheological properties, liquid crystalline polyesters, molecular simulation

Numerical simulation of the mold filling in foam reaction injection molding Dongjin Seo and Jae Ryoun Youn

School of Materials Science and Engineering, Seoul National University, Seoul 151-742, Korea seos@korea.com

Reaction injection molding (RIM) of polymeric foam is a complex process. It consists of chemical reaction, nucleation, bubble growth and mold filling due to self-expansion of the foam. Mold filling is driven by the foam density that is reduced by the bubble growth. In this study, it is assumed that foam is a continuous medium which is characterized by the Newtonian fluid and that variation of foam density is already known. As a basic investigation, an isothermal case is considered. In order to model the process, we developed a numerical method that includes SIMPLER algorithm with the finite concept method (FCM) and proper treatment of the moving boundary.

Keywords: foam molding, finite concept method, reaction injection molding

Direct analysis of entanglements in the atomic structure of high polymer melts

Alfred Uhlherr, Vlasis G. Mavrantzas and Doros N. Theodorou

CSIRO Molecular Science, Clayton 3169, Australia a.uhlherr@molsci.csiro.au

Since new atomistic Monte Carlo simulation techniques now make it possible to quantitatively analyse high polymers at the atomic level, we can use the formalism of Wool (Macromolecules 26 (1993) 1564) to directly calculate the critical entanglement length, Mc, from the average frequency of chain intersections with an arbitrary load-bearing plane. For simulated melts of polydisperse linear polyethylene, this "first principles" approach gives Mc = 3400 g/mol, in good agreement with the experimental viscosity scaling crossover. Furthermore the method yields Mc for individual chains in specified directions, allowing us to confirm that this length is constant (and isotropic) for equilibrium melts of average molecular weight 14000 - 84000 g/mol.

Keywords: molecular simulation, high density polyethylene, critical entanglement molecular weight

Mathematical characteristics of the pom-pom model

Youngdon Kwon and Jae Wook Lee

Sungkyunkwan University, Suwon 440-746, Korea ydkwon@yurim.skku.ac.kr

Mathematical analysis in view of Hadamard and dissipative stabilities has been performed for the pom-pom constitutive equations. It is proved for the differential version that they are globally Hadamard stable except for the case of maximum constant backbone stretch with arm withdrawal neglected, as long as the orientation tensor remains positive definite or the smooth strain history in the flow is previously given. However this model is proved dissipative unstable, since steady shear flow curves exhibit non-monotonic dependence on shear rate. Highly unstable behavior for creep shear flow has also been revealed.

Keywords: pom-pom model, mathematical stability, creep flow

Rheological and mechanical properties of syndiotactic polystyrene/organoclay nanocomposites Cheon II Park, Won Mook Choi, O Ok Park, Jae Gon Lim and Hyun Joon Kim

Department of Chemical Engineering, Center for Advanced Functional Polymers Korea Advanced Institute of Science and Technology Taejon 305-701, Korea mook98@kaist.ac.kr

In this study, we attempted to fabricate the nanocomposite of sPS/clay nanocomposite by melt intercalation. Due to the instability of organic clay at high processing temperature (over 270°C), it is needed to employ the step wise mixing amorphous styrenic copolymers that are miscible with sPS, such as SMA, and SEBS-MA. The microstructures of the nanocomposites depend on the kind of amorphous styrenic polymers. Nanocomposites using SMA have

firmer intercalation structure than those using aPS due to the interaction of maleic anhydride with layer surface of clay. And the exfoliated structure is obtained in nanocomposite using SEBS-MA. The improvement of mechanical properties, morphology and rheological properties of sPS nanocomposites were investigated.

Modelling of reaction injection molding process of phenol-formaldehyde resin filled with wood dust Jae Wook Lee¹, Youngdon Kwon¹ and A I Leonov²,

¹Sungkyunkwan University, Suwon 440-746, Korea ²Institute of Polymer Engineering, The University of Akron, USA ayaz75@mail.skku,ac.kr

In this study, mathematical modelling of reaction injection molding process of phenol-formaldehyde resin filled with wood dust has been performed. Urotropine is used as a curing agent. The filled polymer fluid is assumed to follow the behaviour of power-law liquid. Mathematical modelling of this non-isothermal flow problem with chemical reaction yields a nonlinear partial differential equation that describes the time evolution of pressure distribution (piezoconductivity) along the mold channel, and we have obtained the analytical solution of this equation. Comparison of the theoretical description with experimental data shows qualitative agreement.

Keywords: piezo-conductivity, injection molding, residual stress

Preparation of Metal Film by Spin Coating Method Hak-Ju Kim, Jung-Ho Lee, II-Hyun Sohn, Myoung-Hwan Oh and Kwan-Young Lee

Department of Chemical Engineering, Korea University Seoul 136-701, Korea hakjukim@korea.ac.kr

Commercialized metal films fabrication processes require high vacuum owing to a high manufacturing cost. While, spin coating method is a simple and low cost process. In this work, metal film conductivity was improved by optimizing the preparation procedure. Desired metal was dissolved into aqueous H_2O_2 , spin coated on the Si or SiO_2 surface and finally reduced in H_2 at appropriate temperature. The measured W film resistivity was 12,000 μΩㆍ㎝. By introducing Mo (50 wt%), the resistivity was decreased to 2,000 μΩ ㆍ㎝. Spin coating method was considered to be a promising process for the process cost-down.

Keywords: metal film, spin coating method, resistivity

Study on the Variation of Rheological Properties in the Process of Colloidal Silica Coatings Prepared by Sol-Gel Method

Hyun Uk Kang, Jong Kook Park and Sung-Hyun Kim Department of Chemical Engineering, Korea University Seoul 136-701, Korea hanugil@korea.ac.kr

The rheological properties of silica suspensions modified with

(Glycidoxypropyl) trimethoxysilane (GPS) have been investigated as a function of pH and agitation. GPS was used as a binder in colloidal silica coatings. The suspensions were prepared by adding GPS and Ethylenediamine (EDA) in order to cure the coatings. Colloidal silica coatings were produced by dip coating method in suspensions. At acidic conditions, suspensions showed a Newtonian behavior. After adding EDA, they have shown high viscosity with curing. The viscosity of suspensions at weak acidic conditions was less higher than that at strong acidic conditions. **Keywords:** suspension, sol-gel method, colloidal silica coating

Large amplitude oscillatory shear behavior of polymer solutions: poly (vinyl alcohol), xanthan gum, hyaluronic acid

Kyu Hyun, Sook Hyun Kim, Hyun Ok Park, Kyung Hyun Ahn and Seung Jong Lee

School of chemical Engineering, Seoul Nationa University, Seoul 151-744, Korea

dding@rheopro3.snu.ac.kr

The rheological properties of complex fluids (a fluid system which shows complex behavior due to the strong interactions among its components) differ from those of typical polymer solutions or melts because there exist strong inter or intra interactions. As they attract more attention in these days, it is necessary to understand their behaviors. And it is necessary to classify them because their behavior is quite diverse. Large amplitude oscillatory shear (LAOS) experiment offers a good opportunity. LAOS behavior of hyaluronic acid, poly (vinyl alcohol), xanthan gum solutions has been investigated in this work. We have observed at least three types of behaviors under the LAOS flow environment.

Keywords: complex fluid, LAOS, poly (vinyl alcohol), hyaluronic acid, xanthan gum

Scale up of viscosity measurement of concentrated suspensions from conventional rheometer to stirred tank reactor Ange NZIHOU

Laboratoire de Génie des Solides Divisés, Ecole des Mines dAlbi Albi 81013, France nzihou@enstimac.fr

The Metzner and Otto approach postulated the couette flow analogy in which the flow produced by an helicoidal rubbon impeller inside a stirred tank reactor can be considered to be similar to that produced by a rotating cylinder inside another cylinder. We proposed an approach relating the relative viscosity versus the volume fraction of solids and the shear rate or the shear strain. The results obtained by fitting the viscosity of dilatant suspensions of acrylic cement and the shear thinning suspensions of incinerator fly ash with the proposed model and the modified Krieger and Dougherty model showed a good agreement. The Reynolds number and the power consumption in the reactor was calculated and discussed using this approach.

Keywords: rheology of suspensions, stirred tank reactor modeling

Synthesis of Thermoplastic Nanocomposites by Two-Stage Sonication Process Joung Gul Ryu, Pil Soo Lee, Hyung Soo Kim and Jae Wook Lee

Department of Chemical Engineering, Sogang University Seoul 121-742, Korea seed1224@hananet.net

Thermoplastic nanocomposites based on organically modified montmorillonite (org-MMT) were prepared by ultrasonically assisted polymerization and melt mixing processes. In the first stage, as an attempt to achieve nano-scale dispersion of org-MMT in the matrix polymer, a mixture of a monomer and org-MMT was put under the irradiation of intensive power ultrasonic wave. During the sonication process, the important roles of the ultrasonic wave are two fold. First, it enhances the initiation of polymerization by atomizing the constituent organic molecules. Second, it facilitates the breakup and delamination of org-MMT agglomerates. In practice, it appears that the exfoliated structure was readily formed in the sonicated polymerization process, while such phase transition was rather limited and only intercalated structure was possible in the conventional in-situ polymerization of styrene and org-MMT. The monomers of interest were styrene and methyl methacrylates. In the second stage, the product obtained from the first stage was used as a concentrate for melt mixing with the corresponding matrix polymer under sonication. Again, the imposed ultrasonic wave was expected to act as an effective mixing element to improve the homogeneity of the nanocomposites. The synthesized nanocomposites via two-stage process revealed enhanced thermal stability, mechanical performance and rheological characteristics compare to the conventional methods.

Keywords: nanocomposite, sonication process, melt intercalation

Rheological and thermal properties of long chain branched polypropylene J.H.Yoo, G.J.Nam, J.H.Kim and J.W.Lee

Department of Chemical Engineering, Sogang University Seoul 121-742, Korea jehyuk@sogang.ac.kr

Although PP has many useful properties, its linear chain structure prohibits its wide applications such as thermoforming and foaming process. Introduction of long chain branch onto the PP and improvement of its melt strength will be the attractive alternatives to overcome its shortcomings. We will present here the rheological properties of long chain branched PP compared to that of linear chain structure. Viscoelastic modelings will be added to predict and characterize the rheological properties. Also, crystallization kinetics will be performed to explain the different crystalline structure of these two polymers.

Keywords: polypropylene, long chain branch, rheological properties, crystallization kinetics

Effect of fluid viscoelasticity on the draw resonance dynamics of film casting process

Joo Sung Lee and Jae Chun Hyun

Department of Chemical Engineering, Korea University, Seoul 136-701, Korea

jslee96@grtrkr.korea.ac.kr

The effect of fluid viscoelasticity on the draw resonance dynamics of film casting process has been examined using Phan-Thien Tanner fluid into the governing equations of the process. Whether or not the fluid viscoelasticity stabilizes film casting process has turned out to coincide with whether or not the tension sensitivity decreases with the increasing fluid viscoelasticity. In the extension thickening cases where tension is increased by increasing viscoelasticity, film casting process is stabilized by viscoelasticity while in the extension thinning cases the opposite is true.

Keywords: draw resonance, sensitivity analysis, viscoelasticity

Dense Fly Ash-Water Slurry Transportation with Additive Feeding System for Restarting of Pipeline System

Lei Li, Hiromoto Usui and Hiroshi Suzuki

Department of Chemical Science and Engineering, Kobe University, Kobe 657-8501, Japan 997d912n@y01.kobe-u.ac.jp

The dense slurry transportation technology has some advantages for long distance transportation of fly ash discharged from the coal-fired power stations. This paper proposes a transportation system with additive feeding system for restarting of pipeline system. Rheological characteristics and sedimentation stability of fly ash-water slurry with addition of four kinds of stabilizing additives (S– 194, S–130, CMC and Vanzan) were measured. S-194 is a stabilizer that is chosen for preparing stable fly ash– water slurry. The stable fly ash– water slurries will be filled in the pipe to prevent the sedimentation of fly ash particles before being shut down. The results of the feasibility study show that the transportation cost of the proposed system is a little larger than the system without additive, but it is easy to restart the system.

Keywords: fly ash suspension, slurry, pipeline transportation

Yield stress measurements of Titanium Dioxide particle suspensions

Masanari Ishizuki, Hiromoto Usui and Hiroshi Suzuki

Department of Chemical Science and Engineering, Kobe University, Kobe 657-8501, Japan 0091504n@y00.kobe-u.ac.jp

The study of rheological properties of various suspensions is important. Especially yield stress is important for the industrial using. However, the definition of yield stress is not established yet. To investigate the yield stress, we measured of stress ramp and measurement of initial stress of titanium dioxide suspension

by shear rate and shear stress controlled type rheometer. Also we calculated the yield stress of titanium dioxide suspension by casson plot. From these data, we determined the yield stress of titanium dioxide suspensions and found out the best measurement of the yield stress.

Keywords: rheology, suspension, yield stress

Numerical simulation of viscoelastic flow in expansion/contraction channel

L Saoudi¹ and N Zeraibi²

¹Institut de Physique, Laboratoire de Mécanique des fluids, USTHB Algiers, Algeria

²Faculté des hydrocarbures et de la chimie, Université de Boumerdes

leila_saoudi@yahoo.fr

Numerical simulation of the flow of the Oldroyd-B fluid in expansion/contraction channel has been carried out using the finite difference technique. In discretizing the continuity, momentum and constitutive equations on a uniform grid system, different schemes are used like Upwind difference scheme and Central difference scheme. The effect of fluid inertia and elasticity is also clarified by analyses the distributions of a stream function, a vorticity and a first normal stress for a variety of Reynolds and Weissenberg numbers; where we discuss their effects upon the corner vortex size and the location of the center of rotation. Elasticity has the effect of increasing the upstream corner vortex size, which is opposite to an inertial effect.

Keywords: Oldroyd-B fluid, expansion/contraction channel, effect of inertia, effect of elasticity, UD scheme, CD scheme, Reynolds number, Weissenberg number

Rheological properties of poly(vinyl alcohol)/hyaluronic acid blends

Sook Hyun Kim, Kyu Hyun, Sung Sik Lee, Kyun Hyun Ahn and Seung Jong Lee

School of Chemical Engineering, Seoul National University, Seoul 151-744, Korea sookms@hotmail.com

Bioartificial polymeric materials, which are based on the blends of synthetic and biological polymers, are opening a new class of materials. Rheological measurements of bioartificial materials prepared with poly (vinyl alcohol) (PVA)-sodium borate association as a synthetic component and hyaluronic acid (HA) as a biological component show the strong interaction between the two components. The complex viscosity increases with increasing HA content up to a maximum value, corresponding to a composition of 20% HA, and then decreases with increasing HA content. Without sodium borate, there is little interaction between the components. The case of a composition of 40% HA shows a good property for opthalmological survey.

Keywords: bioartificial polymers, poly (vinyl alcohol), sodium borate, hyaluronic acid

The rheology of bread dough made from four commercial flours

M Keentok^{1,2}, M P Newberry^{1,2}, P Gras^{1,3}, F Bekes^{1,3} and R I Tanner^{1,2}

¹Quality Wheat Cooperative Research Centre Ltd, North Ryde 1670, Australia

²Department of Mechanical and Mechatronic Engineering, University of Sydney, NSW 2006, Australia

³CSIRO Plant Industry, Grain Quality Research Laboratory, North Ryde 1670, Australia

mattik@aeromech.usyd.edu.au

A selection of four commercial flours has been subjected to extensive rheological measurements as part of a comprehensive program of wheat improvement (under the auspices of the Quality Wheat CRC in North Ryde, Sydney). The results have been used to determine which of the many types of rheological measurements provide significant discrimination between various types of modern baker's flours (including biscuit flours) and to procur data suitable for use in mathematical models describing the dough rheology. The rheological measurements undertaken include: oscillatory shear at low amplitude, steady shear at a low shear rate, stress relaxation and extensional viscosity testing. Particular attention was paid to removal of slip. Although oscillatory shear data shows minor differences between these flours, the other tests show significant variations and these provide very good discrimination between the different flour types in comparison with conventional dough testing (e.g. by the extensograph). The current dough rheological measurements provide further insight into molecular structure. In the future, mathematical (constitutive) models will provide a means of predicting processing and baking behaviour of bread dough.

Keywords: bread dough, oscillatory shear, steady shear (viscometry)

Comparison of Cylinder and Cone Geometries for Yield Stress Measurement with the Slump Test Sam Clayton¹, David Boger¹ and Tony Grice²

¹Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia

²Australian Mining Consultants, Melbourne 3000, Australia s.clayton@pgrad.unimelb.edu.au

In industrial applications, the slump test provides a simple means for monitoring the consistency of mineral suspensions. The control variable is the empirical slump height, which is dependent on both material yield stress and density. We propose that the yield stress, a direct material property, is a better control variable. Models relating the slump height to yield stress for cylinder and cone slump tests are compared and evaluated. The investigation clearly shows that the cylinder geometry is more accurate and less complex than the widely used cone geometry.

Keywords: yield stress, slump test, mineral suspension

The Plasticisation Effect of Glycerol on The Gela-

tinisation of Wheat Starch G Nashed, P A Sopade and R Rutgers

Department of Chemical Engineering, The University of Queensland, Brisbane 4072, Australia Genan@cheque.uq.edu.au

The effect of glycerol on the gelatinisation of wheat starch was studied using differential scanning calorimetry (DSC). The water content ranged from 15 - 30% while the glycerol concentration varied up to 85%. The enthalpy of gelatinisation varied from 1.7 - 12.6 J/g of dry starch. The onset and peak temperatures of the gelatinisation endotherm were 54 - 86°C and 60 - 900C respectively, and both water and glycerol significantly affected these. Glycerol behaved as an anti-plasticiser since it generally increased these temperatures. Glycerol is hydrophilic, and it possibly reduced the water available for the starch to gelatinise and hence hindered the gelatinisation process. Sorption data to support this hypothesis are presented.

Keywords: starch, glycerol, gelatinisation

Flow and additive effects on the mesoporous silica structure fabricated by using block copolymer templating

Dae-Geun Choi and Seung-Man Yang

Department of Chemical Engineering, Korea Advanced Institute of Science and Technology, Taejon 305-701, Korea smyang@kaist.ac.kr

In the present study, mesoporous silica structure was fabricated by using triblock copolymer templates. The triblock copolymer was poly (ethylene oxide) (PEO) and poly (propylene oxide) (PPO) and xylene was used to control the pore size. The microstructure of the triblock copolymer was shown to be affected by the additive concentration and the flow intensity. The prepared silica structure was characterized by X-ray diffraction (XRD), transmission electron microscopy (TEM) and N_2 sorption experiment. The prepared mesoporous silica structure showed long-range 2-dimensional hexagonal ordering.

Keywords: mesoporous silica, block copolymers, hexagonal ordering

Applications of rheology in suspension dewatering Shane P Usher, Ross G de Kretser and Peter J Scales

Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia s.usher@pgrad.unimelb.edu.au

Many industrial suspension dewatering operations such as filtration, centrifugation, gravity thickening and tailings dam consolidation can now be predicted by using rheological properties including shear stress versus shear rate behaviour, compressibility and permeability. Only shear behaviour is widely reported with compressibility and permeability often neglected due to a lack of knowledge about how to characterise and use this information. A newly developed and comprehensive set of characterisation techniques are now available. Process equipment operation is modelled from suspension characterisation data and compared with process outputs as an example of how these tools can improve understanding of suspension dewatering operations.

Keywords: suspension dewaterability characterisation, thickener modelling, compressibility, permeability.

Determination of the discrete relaxation spectrum from dynamic moduli using a nonlinear regression method

Gholamhossein Sodeifian and Ali Haghtalab

Faculty of Engineering, Tarbiat Modarres University Tehran, Iran sodifig@net1cs.modares.ac.ir

The relaxation spectrum has an important role in analysing the experimental results. The most common procedure is to use data from a small-amplitude oscillatory shear experiment. However, this is an ill-posed problem and its numerical solution is along with difficulties. The determination of the discrete relaxation spectrum by a linear regression approach is widespread in the literature. In this work, a nonlinear regression method based on Marquardt-Levenberg procedure is applied. The method has been tested using several experimental results such as HDPE, PB and PS. It has been shown that in comparison with the other methods, the present approach is more efficient and it was found to give an excellent fit with the fewest possible parameters.

Keywords: rheology, nonlinear regression, relaxation spectrum

Ternary Blended Polyethylene Films: A Study on its Mechanical and Thermal Properties Rahul Kumar Gupta¹ and Deepak Srivastava²

¹Department of Chemical & Metallurgical Engineering, RMIT University, Melboune 3001, Australia

²Deptartment of Plastic Technology, H. B. Technological Institute, Kanpur 208 002 (U.P.), India deepak_sri92@rediffmail.com

Ternary blended of film samples of LDPE, HDPE and LLDPE were prepared by blown film extrusion technique. The structural changes, due to formation of oxygenated and unsaturated groups during extrusion, has been studied by infrared (IR) spectroscopic analysis. This change in structure was further studied to correlate various physico-mechanical and thermal properties of the film samples. The tensile strength has been found to increase upto 25 weight percent HDPE addition in LDPE and LLDPE and decreased thereafter. The elongation at break decreased upto 20 weight, percent addition of LDPE/LLDPE blends and then increased. A trend similar to tensile strength has also been observed for impact strength. The initial degradation temperature (IDT) has been evaluated for blend composition having LDPE: LLDPE;HDPE = 50:25:25 (A-500) from thermogravimetric analyzer (TGA) and it was found to be 310°C. Differential scanning calorimetric (DSC) analysis was performed for all film samples to investigate the effect on melting t

Keywords: ternary blend, tensile strength, impact strength, initial degradation temperature (IDT), melting temperature, morphology

Synthesis polyaniline-surface modified clay composites for application electrorheological fluids Jong Hyeok Park, Yong Taik Lim and O Ok Park

Center for Advanced Functional Polymer (CAFPoly), Department of Chemical Engineering, Korea Advanced Institute of Science and Technology, Taejon 305-701, Korea oopark@kaist.ac.kr

We synthesized polyaniline (hereafter PANI) / organoclay (aminosilane surface treated) nanocomposite particles and prepared electrorheological (ER) fluids by dispersing the particles in silicone oil. Distinct enhancement in yield stress was observed due to the presence of PANI coated clay particles. The effects of delaminated clay to the ER yield stress were investigated and compared with other ER fluid systems which use PANI particles only or simple intercalated PANI/clay nanocomposite.

Keywords: electrorheology, conducting polymer/clay nanocom posite, field responsible fluids

Transportation of ice slurry to reduce the pumping power for energy saving cooling system Hiromoto Usui, Hiroshi Suzuki and Poly R Modak

Department of Chemical Engineering, Kobe University, Kobe 657-8501, Japan usui@cx.kobe-u.ac.jp

Adding surfactants and auxiliary salt controlled the diameter of ice particles suspended in chilled water. The ice – water slurry, thus prepared, was forced to flow in a round tube in turbulent condition. Volume fraction of ice, particle size distribution, slurry viscosity and pressure drop in a pipe flow were measured. Experimental results of pressure drop showed a drastic reduction of pumping power, although the viscosity measured by B-type rheometer showed much higher value compared from water viscosity. Possible way to reduce the pumping power to transport slurries is suggested in this paper.

Keywords: suspension, ice particle, air conditioning system

A novel method to measure the melt viscosity: the screw rheometer

Myung-Ho Kim, Young-Tak Oh, Shi-Ho Lee and Soon-Yong

LG Chemical Ltd/Polymer Processing Technology Team at Tech Center Science Town, Taejeon 305-343, Korea mhkimt@lgchem.co.kr

An experimental study was carried out to use the Screw Rheometer to measure the viscosities of rubbery material and commercial grade LDPE. The 45 mm diameter single screw extruder

was modified to build the Screw Rheometer by designing a special die head, and the pressure transducers on the different barrel locations. Comparison with commercial capillary rheometer results for LDPE showed good agreements for various temperatures. For the rubbery materials which show discrepancy in the capillary type rheometers, melt viscosities were measured using the Screw Rheometer and compared with the capillary rheometer result.

Keywords: screw rheometer, viscosity, extruder

An overview on the swirling flow of non-Newtonian fluids

Jason R Stokes

Unilever Research Colworth Sharnbrook, Bedford MK44 1LQ, United Kingdom

jason.stokes@unilever.com

The behaviour of non-Newtonian fluids in an enclosed cylindrical vessel with a rotating lid has been examined over the last 30 years both experimentally and theoretically. Early experimental work involved the use of shear-thinning elastic fluids where it was difficult to separate the effects of elasticity on the flow behaviour. However, recent investigations have been performed utilising a range of constant viscosity elastic fluids with and without the presence of inertial forces in the system. This has enabled a better understanding of the behaviour of non-Newtonian fluids in swirling flow from which to base numerical predictions as a test of non-Newtonian constitutive models in a complex yet well defined three-dimensional geometry.

Keywords: viscoelastic, elastic instability, swirling flow

Melting phenomena and mechanism in polymer processing equipment Myung-Ho Kim¹ and Costas G. Gogos²

¹LG Chemical Ltd Tech Center Science Town, Taejeon, Korea ²Polymer Processing Institute, Newark, New Jersey, U S A mhkimt@lgchem.co.kr

The research work presented here examines the heating and melting phenomena taking place, when individual polymer particulates or compacted polymer particulate systems are subjected to stresses which force them to deform and flow. The heating/melting behavior in compression experiments of single polymer cylinders and in co-rotating twin screw extruders was examined. Different polymers and different polymer particulate solid systems were used, over a range of processing conditions. The results of this work shed light on the important roles that solid dissipative deformation and interparticle frictional phenomena play in generating the heat necessary to melt polymer particulate systems. *Keywords**: dissipative mixing melting, plastic energy dissipation, melting mechanism

Effect of degree of saponification on the rheological properties of syndiotactic poly (vinyl alcohol)/

water solution

Bong Shik Kim¹, In Seok Seo², Byung Chul Ji², Won Sik Yoon³ and Won Seok Lyoo³

¹School of Chemical Engineering and Technology, Yeungnam University, Kyongsan 712-749, Korea

²Department of Dyeing and Finishing, Kyongpook National University, Taegu, Korea

³School of Textiles, Yeungnam University, Kyongsan 712-749, Korea

kimbs@yu.ac.kr

Four kinds of poly (vinyl alcohol) (PVA) with assigned degrees of saponification, from 93.1 to 97.5% were prepared by copolymerisation of vinyl acetate and vinyl pivalate, followed by saponifying the corresponding poly (vinyl acetate)/poly (vinyl pivalate) copolymer, respectively. PVA with higher degree of saponification shows more shear thinning at similar molecular weight of polymer, suggesting that PVA molecules are more readily oriented as degree of saponification increases. This may provide indirect evidence of the spontaneous in situ orientation of polymer molecules at the late stage of saponification. Yield stress is higher for the polymer with higher degree of saponification at similar molecular weight of polymer. This indicates that more domains with internal orders are produced at higher saponification. These facts result from increase in stiffness of polymer molecules with proceeding the saponification reaction.

Keywords: degree of saponification, <u>syndiotactic</u> poly (vinyl alcohol), rheological properties

Polyethylene flow prediction with a differential multi-mode Pom Pom model

R P G Rutgers¹, N Clemeur¹ and S Muke²

¹Department of Chemical Engineering, The University of Queensland, St Lucia 4072, Australia

²Department of Chemical and Metallurgical Engineering, RMIT University, Melbourne 3000, Australia

We report the first steps of a collaborative project between the University of Queensland, Polyflow, Michelin, SK Chemicals and RMIT University on simulation, validation and application of a recently introduced constitutive model designed to describe branched polymers. Whereas much progress has been made on predicting the complex flow behaviour of many in particular, linear polymers, it has been proven difficult to predict simultaneously shear thinning and extensional strain hardening behaviour using traditional constitutive models. Recently a new viscoelastic model based on molecular topology was proposed by McLeish and Larson[1]. We explore the predictive power of a differential multi-mode version of the pom-pom model for the flow behaviour of two commercial polymer melts: a (long-chain branched) low-density polyethylene (LDPE) and a (linear) high-density polyethylene (HDPE). The model responses are compared to elongational recovery experiments published by Langouche and Debbaut[2], and start-up of simple shear flow, stress relaxation after simple and reverse step strain experiments carried out in our laboratory. The

model performance is assessed in planar contraction flow in comparison with the well-established Phan Thien-Tanner and KBKZ models.

1. McLeish, T C B and R G Larson, J. Rheol, 1998. 42(1): p 81-110

Numerical Investigation of Interface Deformation in Stratified Coextrusion Flow of Viscoelastic Fluids

Seong Jae Lee¹, Ki Byung Sunwoo², Kyung Hyun Ahn² and Seung Jong Lee²

Department of Polymer Engineering, The University of Suwon, Kyunggi 445-743, Korea

²School of Chemical Engineering, Seoul National University, Seoul 151-742, Korea

sjlee@mail.suwon.ac.kr

Interface deformation in coextrusion process directly depends on the rheological properties of fluids. Experimental and theoretical investigations have so far revealed that the viscosity difference and the difference of the second normal stress differences between fluids are the controlling factors of this phenomenon. In this study, we performed three-dimensional numerical simulation on stratified coextrusion flow of viscoelastic fluids through a rectangular die. After fitting the viscosity data and tuning the relevant parameters of constitutive models which control cross-sectional interface profile and degree of encapsulation, satisfactory results can be obtained in accordance with the experimental results from other investigators.

Keywords: coextrusion, numerical simulation, three-dimensional flow

Effect of macromolecular properties on shear rheology of low-density polyethylene (LDPE) R K Gupta, I Ivanov, A Chryss and S N Bhattacharya

Department of Chemical and Metallurgical Engineering, RMIT University, Melbourne 3000, Australia Rahul.gupta@rmit.edu.au

Low-density polyethylene is a versatile polymer that finds use in various products. Variation of properties in the polymer is caused mainly by its high degree of long chain branching (LCB). This work is aimed at studying how the rheological behaviour of LDPE changes with various degree of long chain branching and relate with molecular weight, molecular weight distribution, polydispersity and branching index obtained from high temperature GPC. Rheological measurements were performed using Dynamic Stress Rheometer RMS-605, investigating both dynamic and steady rate moduli. Results showed that increase in degree of long chain branching reduces zero shear viscosity but increases the activation energy obtained from shear rheology.

Keywords: polydispersity index, branching index, low-density polyethylene

Extracting the memory and relaxation functions of viscoelastic fluids from small amplitude oscillatory shear data

Y Leong YEOW

Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia yly@unimelb.edu.au

The problem of extracting the memory function of viscoelastic fluids from oscillatory shear data is formulated as an inverse problem of solving two integral equations of the first kind. A procedure based on Tikhonov regularization is used to solve these equations. The resulting memory function is then integrated to give the relaxation function. This procedure is used to process the oscillatory shear data of a polymer solution and a melt. The relaxation functions thus obtained are compared against published results. These examples show that Tikhonov regularisation is a reliable method for obtaining the material functions of viscoelastic fluids.

Keywords: relaxation function, oscillatory shear test, Tikhonov regularisation

Estimation of polydispersity index of branched polypropylene by rheological techniques D Roy, S N Bhattacharya, R K Gupta, H C Lau and M OShea

Department of Chemical and Metallurgical Engineering, RMIT University, Melbourne 3000, Australia Debashis.Roy@rmit.edu.au

The polydispersity index (PI) of polypropylene (PP) obtained from the crossover point of shear storage modulus (G) and loss modulus (G") by using the following equation:

 $PI = 10^5 (Pa)/G_c$

where $G_c = G = G''$ at the crossover frequency. Rheological properties such as the zero shear viscosity (η_0) and the fluidity difference $\Delta \phi$ (i.e. $1/\eta - 1/\eta_0$) between the Newtonian and non-Newtonian conditions have been applied for investigations of branched structures of PP. Branching parameters that characterize the long chain branching (LCB) of macromolecules have been determined using the multivariable power function (MVP) for the dependence of η_0 and $\Delta \phi$ on MWD and LCB. One of the exponents of the MVP function distinguishes linear from the branched structures within the modified PP. Virgin and peroxide modified PP samples were analysed at four different temperatures (190, 200, 210 and 230°C). The information on branching was also obtained from the calculation of flow activation energy from Arrhenius plot. This trend was correlated with the branching index obtained from the MVP function. These results were also confirmed by relaxation times obtained from the dynamic data.

Keywords: polydispersity index, branching index, relaxation time, polypropylene

Gaussian Approximation for Hookean Dumbbells with Hydrodynamic Interaction and Excluded Volume

Ravi Prakash, Prabhakar Ranganathan

Department of Chemical Engineering, Monash University Clayton 3168, Australia

ravi.jagadeeshan@eng.monash.edu.au

A suspension of non-interacting Hookean dumbbells is used to model a dilute solution of polymers in a good solvent by accounting for both excluded volume (EV) and hydrodynamic interactions (HI). Material functions in simple shear flows have been obtained by assuming that the non-equilibrium connector vector distribution function is Gaussian. These approximate material functions have been compared with exact results obtained by Brownian dynamics simulations. The predicted viscometric functions are seen to undergo more pronounced shear thinning when both HI and EV are present, than when only the former is present, in qualitative agreement with experimental observations.

Keywords: dilute polymer solutions, hydrodynamic interactions, excluded volume

Rheological and Mechanical Properties of Abs/pc Blends

M.M.K.Khan¹, R.F.Liang², R.K.Gupta²

¹James Goldston Faculty of Engineering and Physical Systems Central Queensland University, Rockhampton 4702, Australia ²Department of Chemical Engineering, West Virginia University Morgantown, WV-26506, USA m.khan@cgu.edu.au

Acrylonitrile-Butadiene-Styrene (ABS), Polycarbonate (PC) and their alloys are an important class of engineering thermoplastics that are widely used for automotive industry, computer and equipment housings. PC is a homogeneous, single phase polymer while ABS is a heterogeneous two-phase terpolymer consisting of rubber phase (PB, BS, BA) as a dispersed phase surrounded by a continuous plastic phase (PS, AS). Blends of virgin ABS and virgin PC at five different compositions, namely, 15%, 30%, 50%, 70% and 85% by weight were prepared and characterised by rheological and mechanical measurements. Rheological properties of these blends in steady, oscillatory and transient step shear were measured on a Rheometrics Mechanical Spectrometer RMS800. Mechanical properties, namely, tensile strength, elongation-at-break were determined on Instron 8501 and Izod impact strength was evaluated on Satec Impact Tester. The results show that PC behaves relatively Newtonian but ABS shows a significant shear thinning effect. The rheological response of ABS-rich blends shows a similar trend to that of ABS, while PC-rich blends, namely 0% and 15%, follow a nearly Newtonian behaviour. However, at a fixed shear rate or frequency, the steady shear or the dynamic viscosity varied respectively in a non-monotonic manner with composition. Except for 15% blend, the viscosities of other blends fall into a narrow band indicating a wide-operation window of varying

blend ratio. The blends exhibited a lower viscosity than either of the two pure components. The other noticeable feature was that the blends at 70% and 85% ABS content had a higher G than pure ABS, indicating an enhancement of elastic effect. The tensile and impact properties of these blends were also evaluated and the results indicate that the processability of PC is improved by adding ABS. The tensile yield strength of the blends follows the rule of mixtures while the elongation-at-break and the impact strength do not obey the rule of mixtures.

Numerical simulation of high Weissenberg number problem in a 4:1 planar contraction flow Seung Jong Lee, Ju Min Kim and Kyung Hyun Ahn

School of Chemical Engineering, Seoul National University Seoul 151-744, Korea silee@plaza.snu.ac.kr

We present a new numerical algorithm based on fully implicit 4-step fractional step method (FSM) with equal-order linear interpolation function. We incorporate the stabilizing techniques such as DEVSS-G (discrete elasto-viscous split stress)/SUPG (streamline upwind Petrov-Galerkin) and DEVSS-G/DG (discontinuous Galerkin) to enhance the convergence. This algorithm has been applied to 4:1 planar contraction flow. Converged solution with FSM + DEVSS-G/DG was obtained up to as high as We = 6 surpassing any previous results. We could observe the collision of corner and lip vortices, followed by a big vortex. It means that the lip vortex enhancement is not a 3-dimensional phenomenon, and the Oldroyd-B model can predict such a complex phenomenon in a 2-dimensional planar contraction flow simulation.

Keywords: high Weissenberg number problem, 4:1 contraction flow, fractional step method, DEVSS, DG

Measurements of fluid model parameters of PET for stretch blow molding simulation Hern-Jin Park, Sangyup Baik and Jae Wook Lee

SK Chemicals Company Ltd, Suwon 440-745, Korea hjpark@skchemicals.com

A process of PET stretch blow molding can be simulated by using multi-mode viscoelastic fluid model. In this work, linear spectrum of a PET was determined using DMTA experiments and the results have been compared with those obtained from large deformation experiments of circular plate using a plug. In both methods, to get the material properties at an amorphous state, the experiments have been carried out at slightly higher temperature than Tg and extrapolated to the typical processing temperature using the WLF equation. A use of the multi-mode viscoelastic model obtained has allowed to simulate successfully the PET stretch blow molding process.

Keywords: blow molding, elongational properties, PET

Macromolecular Dynamics in Shear at Concentrations above Critical Overlap

Yalin Wei and Dave E Dunstan

CRC for Bioproducts Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia davided@unimelb.edu.au

The shear induced orientation and deformation of polymer coils in concentrated solution have been investigated by using the optical absorption properties of the polymeric chromophore diacetylene 4-butoxycarbonylmethlurethane (4BCMU). The orientation and deformation of this polymer is measured in shear by monitoring the magnitude and spectral shift of the absorption respectively. Measurements have been performed at three concentra-tions above the critical overlap concentration, C*. The normalised changes in extinction coefficient are the same within experimental error at the three concentrations. At low shear the orientation of the polymer backbone occurs parallel to the shear to decrease with increasing shear rate to align perpendicular to the shear at rates higher than 500 s⁻¹. The measured spectral shift in shear shows that the distribution of conjugation lengths decreases systematically with increasing shear rate. The data is explained by hypothesising that at low shear the polymer segments align with the shear direction while at high shear rates the polymer segments roll with their main axes perpendicular to the shear direction.

The Influence of Die Geometry and Extrusion Rate on the Melt Strength Measurement of Polypropylene

H Č Lau, S N Bhattacharya, R K Gupta and M OShea

Rheology & Materials Processing Centre, Department of Chemical & Metallurgical Engineering, RMIT University, Melbourne 3000, Australia

andro.lau@rmit.edu.au

In polymer processes such as blow film extrusion and thermoforming, the processing behaviour of a polymer can be related to its melt strength. Melt strength is defined as an extensional force required to rupture a melt strand and it can be measured by using a Göttfert "Rheotens" Melt Strength Tester. It is recognised that melt strength measurement does not give a well-defined rheological property. In melt strength measurement, the polymer melt has to be extruded in an extruder where both shear and extensional deformation history is present in the melt. Depending on the die geometry used in the extrusion, different molecular orientation can be induced in the melt. For a given die geometry, the rate of extrusion can also alter the orientation in the polymer melt exiting from the die and subsequently affects the melt strength of the polymer. The melt strength of conventional polypropylene (PP) is usually low and the variation of die geometry may not show any significant change in its melt strength. However for polymers such as high melt strength (HMS) PP, the effect die geometry can be become important since the polymer has higher elasticity compared to the conventional PP. In this work, dies with different L/D ratios and entrance angles have been used to study the melt strength of conventional and HMS PP. It was found that the melt strength of PP decreases as the L/D ratio increases due to the stress relaxation of the polymer. For a given die geometry, melt strength increases as the extrusion rate increases. Higher melt strength was also observed when a die with wider entrance angle was used. The complexity of achieving a well defined extensional rheological property from melt strength measurement is highlighted in this work.

Keywords: melt strength, polypropylene

The Measurement of Viscosity in a Gelling Suspension

A F Collings and J A Sor

CSIRO Telecommunications and Industrial Physics Lindfield 2070, Australia tonyc@tip.csiro.au

The rate of change of viscosity in a gelling suspension offers inprinciple information on the structure of the gel which ultimately forms. Since viscometric techniques are frequently used to characterise gel structure, one must ensure that the technique does not itself influence this structure as a consequence of the velocity gradient which it employs. This paper deals with the use of the Love acoustic wave device for measuring changing viscosity in a suspension undergoing gelation. The advantage of this device is that it generates only microscopic gradients and shears. Its suitability is demonstrated for gelation of gelatin and laponite suspensions. Keywords: gelation, acoustic wave devices, near-surface

viscosity, laponite

Instabilities and other problems in parallel plate rheometry

M.Keentok

School of Aerospace, Mechanical and Mechatronic Engineering, University of Sydney, Sydney 2006, Australia mattik@aeromech.usyd.edu.au

The experimental rheologist faces many practical problems in the laboratory, and not the least of these are various flow instabilities which confound any measurements. A well known instability is shear fracture or edge fracture which will be briefly described. This instability now has a well-established theory (Tanner and Keentok, 1983) which has been verified with experimental data and a computational study. This theory and experimental work provide some guidelines for avoidance of edge fracture. Another instability, not previously described in the parallel plate, has been seen also and this is similar to a 'wavy' instability in Couette flow. Examples of this wavy instability will be shown. This instability appears to occur in Boger fluids hich have a small or zero second normal stress difference. Another problem which is often faced by rheologists working with suspensions, is the phenomenon of slip. Slip may also be a factor in melt fracture, which occurs in polymer melts. Slip is a problem in dough rheology and can be minimised, if not eliminated, by the use of sandpapered plates. Some theory will be introduced to show the effect of plate roughness on slip. Measurements on sandpaper roughness have been made and, together with the known particle size distribution

in bread dough, these support the experimental observation that bread dough is not slipping in the parallel plate rheometer. *Keywords*: instability, rheometry, slip

Rheological Characterisation of Rapid Settling Slurries

T.J. Akroyd¹, Q.D. Nguyen¹ and N. Vagias

¹Department of Chemical Engineering, The University of Adelaide, Adelaide 5005, Australia tjakroyd@chemeng.adelaide.edu.au

Mineral solids are usually processed, produced or handled in the form of two-phase slurries. The ability to handle, process and optimise equipment performance critically depends on the viscous and flow behaviour of the slurries. We have previously reported on the development of an on-line continuous flow rheometer based on the principles of helical flow. In this paper we continue to discuss the development and present results obtained for a range of fluids including real mineral slurries. The rheological results from the continuous flow rheometer are compared with results from standard geometries (cone and plate and concentric cylinder) and show excellent agreement for the various fluids tested.

Keywords: flow rheometer, on-line viscometer, mineral slurry

Structure for hydrophobically modified hydroxyethyl cellulose in the presence of an anionic surfactant

Viyada Tirtaatmadja, Sam Gason and Justin Cooper-White Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia viyada@unimelb.edu.au

This study investigates the interactions between hydrophobically modified HEC and the surfactant SDS. Solutions of 0.5% hmHEC (above its cac) show enhanced shear viscosity and elastic modulus when mixed with SDS at intermediate concentrations. The solutions also show shear-induced thickening, followed by shear-thinning, while further increase in the surfactant concentrations causes a decrease in both the viscous and elastic moduli. The enhancement in rheological property is due to the formation of mixed micellar junctions of polymer hydrophobes and the surfactant (hydrophobic) tail, which are broken down at high applied stress. From the elastic modulus data the effective polymer length between junctions may be estimated and the structure of the complex elucidated.

Keywords: polymer-surfactant complexes, shear-induced thickening

Compressional Rheology of Suspensions Peter J Scales

Department of Chemical Engineering, The University of Melbourne, Victoria 3010, Australia peterjs@unimelb.edu.au The measurement of the shear rheology of concentrated particle suspensions is common. For coagulated suspensions of particles, these measurements give rise to behaviour ranging from Newtonian flow curves at low solids concentrations to yield stress and shear thinning behaviour at higher concentrations. The yield stress is a reflection of the fact that for concentrated coagulated particle suspensions, there is a net attractive force between the particles of the suspension that must be overcome for flow to occur. The role of solution conditions and additives such as dispersants in modulating the rheology has been extensively studied. In the case of compressive as distinct from shear forces, the measurement of the rheology is restricted to coagulated suspensions at concentrations above the percolation point of the network. The nature of the network failure and the role of additives and solution conditions are less well understood. A new filtration device has been commissioned at the University of Melbourne that now makes the measurement of compressional rheology fast and reproducible. Results show that many of the trends displayed by the shear yield stress of a suspension are mimicked in the compressional properties although the failure mechanism in the presence of additives is not as well understood.

Effects of rotating speed on the patterns of particle segregation in a rimming flow of polymer solution Sun Hyuk Bae and Do Hyun Kim

Department of Chemical Engineering, Korea Advanced Institute of Science and Technology, Taejon 305-701, Korea semine@kaist.ac.kr

In recent experiments, neutrally buoyant particles in a horizontal cylinder partially filled with a highly viscous Newtonian fluid segregate into bands along the wall. In this study we performed experiments of particle segregation in a non-Newtonian polymer solution and investigated the effects of rotating speed on the patterns of particle segregation. The mono-dispersed spherical polymethylmethacrylate (PMMA) particles were dispersed uniformly in the weakly shear-thinning polymer solution prepared by dissolving polyacrylamide in a mixture of glycerin and ethylene glycol. We found that the shape of bands and the effects of rotating speed showed different behavior from the case of Newtonian fluid.

Keywords: particle segregation, rimming flow, polymer solution

Static measurement of yield stress using a cylindrical penetrometer

P H T Uhlherr, J Guo, T-N Fang and C Tiu

Department of Chemical Engineering, Monash University Clayton 3168, Australia

A novel and simple method using a cylindrical penetrometer for the measurement of yield stress has been developed. The principal of this technique is based on the measurement of the static equilibrium of a falling penetrometer in a yield stress fluid. The yield stress is simply determined by a balance of forces acting on the penetrometer. The yield stresses of Carbopol gel and TiO_2

suspensions have been measured using this method. The results are in reasonable agreement with the values from conventional methods. The effects of the dimensions and weight of the penetrometer have been examined. The long-term creep was also observed. It was found that the effect of creep on static equilibrium is negligible after a minimum measuring time. The cylindrical penetrometer technique promises to be a simple, quick and reliable static method for the measurement of yield stress.

Calibration of a commercial instrumented measuring kneader for rheological applications T Kealy and C Tiu

Co-Operative Research Centre for Clean Power from Lignite, Department of Chemical Engineering, Monash University, Victoria 3800, Australia

tim.kealy@eng.monash.edu.au

In the case of some highly viscous fluids rotational viscometers

are not suitable for rheological characterisation. Due to their capacity for generating and maintaining high torque and/or high rates of rotation, instrumented kneaders and mixers can often engender shear rates in excess of those of conventional rotational viscometers. The problem facing users of these mixers lies in relating rate of rotation and torque data to shear rate and shear stress respectively. If it were possible to obtain such relationships, useful rheological data could be generated from mixer data. This work outlines the experimental and analytical techniques required for converting pertinent data from the IkaVisc MKD 0.6-H60 instrumented kneader into useful rheological quantities. The kneader is calibrated using a variety of Newtonian fluids and the calibration successfully tested on highly shear thinning solutions. A number of assumptions and empiricisms are utilised for this approach. The approximate nature of the technique is offset by furnishing further capacity for rheological data collection to the interested scientist or engineer.

Keywords: rheological calibration, mixing kneader, rotational viscometer