Moldflow Technology

Recent Developments & Data Requirements

NPL March 12 2008



Who we are Global Operations



Moldflow Products - Core Modules

- Injection moulding:
 - -MPI/Flow
 - -MPI/Cool
 - -MPI/Warp





Other Simulation Applications

- Design of Experiments
- Mould core deflection
- 2-shot, Co-injection
- Gas assist
- Injection-compression
- Insert overmoulding
- Micromoulding
- Rubbers & Thermosets, incl warpage
- Liquid Crystal Polymers
- MuCell
- Birefringence
- Interface to FEA (structural loading)



Fill Pattern Verification

Moldflow prediction for flow pattern near end of fill



Short shots to show actual flow pattern near end of fill







Solver Improvements

- Gravity effects
 - For low viscosity materials
- Polymer jetting flow
 - Causes flow marks on surface
 - Polymer jet buckles, touches mould and cools



Compressive Heating Added

- Compressive heating added to energy equation for fluid flow
- Melt temperature will increase as the material gets compressed
- Generally pressures will be 4% to 5% lower than before





Measured Melt-Mould Heat Transfer Coefficient

- Thermal contact resistance measured during molding cycle
- HTC = 1/TCR
- Delaunay, Le Bot et al. Poly.Eng.Sci 40 (1682-1691)



3-Stage Heat Transfer Coefficient (HTC)

- Flow Solvers now use 3-stage HTC
- Defaults
 - 5000 W/m² Filling
 - 2500 W/m² Packing
 - 1250 W/m² Detached (pressure = 0)

Mold-melt Heat Transfer Coefficient (HT)	C) values ———	
Filling	5000	W/m^2-C (500:)
Packing	2500	W/m^2-C (500:)
Detached	1250	W/m^2-C (500:)





Test Resources



- Visco-elastic
- Thermoset Chemo-Rheometry
- Shrinkage for fibre materials
- No flow temperature for LCP's

Melbourne + Ithaca, NY Ithaca, NY, US **Injection Molding** Rheometry Shrinkage testing **Pressure Volume** Temperature Thermal conductivity Capillary **Differential Scanning** Calorimetry Solid Density Shrinkage Measurements pvT for Moisture Measurement **Material Conditioners Environmental Control**

- **Mechanical** Properties
- **Twin Bore** Rheometer
- Shrinkage for nonfibre materials
 - Thermosets



International Standards

Injection Molding Rheology:

- ASTM D5422 Standard Test Method for Measurement of Thermoplastic Materials by Screw-Extrusion Capillary Rheometer
- ASTM D3835 Standard Test Method for Determination of Properties of Polymeric Materials by Means of a Capillary Rheometer
- ISO-11443 Plastics Determination of the fluidity of plastics using capillary and slit-die rheometers

Thermal Conductivity:

• ASTM D5930, Standard Test Method for Thermal Conductivity of Plastics by Means of a Transient Line-Source Technique

Differential Scanning Calorimetry:

- ASTM E1269 Determination of Specific Heat Capacity by Differential Scanning Calorimeter
- ASTM D3417 Enthalpies of Fusion and Crystallization of Polymers by Differential Scanning Calorimeter
- ASTM D3418 Transition Temperatures of Polymers by Differential Scanning Calorimetry

Mechanical Properties:

- ASTM D-638 Tensile Properties of Plastics
- ASTM E-132 Poisson's Ratio at Room Temperature

Coefficient of Thermal Expansion:

• ASTM D-696 Coefficient of Linear Thermal Expansion of Plastics



American Association for Laboratory Accreditation



A2LA has accredited

MOLDFLOW PLASTICS LAB Ithaca, NY

<u>Test Method</u>	Test
ASTM D618	Conditioning Plastics for Testing
ASTM D696	Coefficient of Linear Thermal Expansion of Plastics (0°C to 60°C only)
ASTM D792	Density and Specific Gravity (Relative Density) of Plastics
ASTM D3417	Enthalpies of Fusion and Crystallization of Polymers by Differential Scanning Calorimetry (DSC)
ASTM D3418	Transition Temperatures of Polymers by Differential Scanning Calorimetry (DSC)
ASTM D3835	Determination of Properties of Polymeric Materials by Means of a Capillary Rheometer
ASTM D5930	Thermal Conductivity of Plastics by Means of a Transient Line-Source Technique
ASTM E1269	Determining Specific Heat Capacity by Differential Scanning Calorimetry (DSC)
QOP-05	Pressure-Volume-Temperature Test





Capillary rheometers

- Rosand RH-7
 - Classic method (offline)
 - Reservoir/Plunger
 - Long residence times
- IMR
 - Moulding machine method (online)
 - Charge/Shutoff Screw
 - Short residence times
 - Suitable for high performance materials





Modified Cross-WLF model

- Cross model captures the shear rate sensitivity of most material families
- WLF equation captures exponential-hyperbolic temperature sensitivity depending on the magnitude of T-T*



where:

- T* = D2 + D3P
- η is Viscosity (Pa. sec.)
- $\dot{\mathcal{Y}}$ is Shear Rate (1/sec.)
- T is Temperature (deg.K)
- P is pressure (Pa)
- Unknowns: D1, D2, D3, A1, A2, Tau*, n

•
$$A2 = A2^{\sim} + D3P$$





Shrinkage Testing & Warpage Coefficients



Shrinkage test facilities - ensures accurate shrinkage predictions

	Rec	ommended Pro	cessing	Rheological Proper	ties	Thermal Properties	PVT Properties
Mechanical Prop	erties	Shrinkage	Properties	Filler Properties	M	uCell ® Material Properties	Optical Properties
Shrinkage model							
Corrected residua	in-mold str	ess (CRIMS)		iew model coefficients			
)bserved nominal	shrinkage						
arallel	0.4	62	%				
erpendicular	0.4	91	%				
) bserved shrinkag	e						
Ainimum Parallel	0.2	154	%				
Aaximum Parallel	0.7	69	%				
Minimum Perpendi	cular 0.2	33	%				
Maximum Perpend	cular 0.7	957	%				
A2 0 A3 0 A4 1 A5 0	.034144 .00121 .03659 .061508 .0007	nge solver para	ameters to be a	consistent with CRIMS m	odel)		
A6 0 Use CRIMS	majo (ond						



Thermal Conductivity K-System II



Single Point Thermal Data

Mechanical Propertie	s Shrinkage Pro	operties Filler Properties	MuCell Material Properties	Optical Properties
Description	Recommended Proce	ssing Rheological Prop	erties Thermal Properties	PVT Properties
pecific heat data				
Temperature (T) C	Specific heat (Cp) He J/kg-C	eating/cooling rate C/s		
250 View specifi	1481	-0.1667	Pl	ot specific heat data
hermal conductivity da	ata			5
Temperature (T) C	Thermal conductivity (W/m-	c) Heating/cooling rate C C/s		
250	0.2	7 0		



Multi Point Thermal Data

Thermoplastics material

Me	echanical Propert	ies	Shrinkage	Properties	Fille	er Pi
D	escription	R	ecommended Pr	rocessing	Rh	eolo
Spe	cific <mark>heat data</mark>				1.11	
	Temperature (T) Sp	ecific heat (Cp) J/kg-C	Heating/cod	oling rate C/s	
1	6	5	1625.9		-0.1667	
2	10	D	1897		-0.1667	
3	11	5	2160		-0.1667	
4	12	0	2471.2		-0.1667	
5	12	5	4640.7		-0.1667	
6	13	0	11397		-0.1667	
7	13	5	4432.1		-0.1667	
8	14	0	2045.6		-0.1667	
9	14	5	2044.4		-0.1667	
10	15	5	2075.1		-0.1667	
11	19	5	2175.3		-0.1667	
12	24	D	2256.6		-0.1667	



Cooling Uses Multi-Point Thermal Data

- Now the cooling solver uses multi-point thermal data for heat flux calculations in the part
- Results typically will have only a subtle change







Improving Simulation for LCP's

 Correct selection of Melt-Mold Heat Transfer Coefficient is significant in LCP materials

ïlling	5000	W/m^2-C (500;)
Packing	2500	W/m^2-C (500:)
etached, cavity side	1250	W/m^2-C (500:)
)etached, core side	1250	W/m^2-C (500:)



LCP - Unusual behaviour at low rates

LCP - "three region" flow

Guo, T., Harrison, G.M., and Ogale, A.A., "Rheology and microstructure of thermotropic liquid crystalline polyesters," Antec (2001).



LCP - Unusual behaviour at high rates

 There is suggestion of a plateau in the data at shear rates > 1,000,000/s



LCP - Complex temperature dependence



• Y.Fan, S.Dai and R.I. Tanner; Korea Australia Rheology Journal **15** (2003) 109



The Matrix Model

 Can capture unusual transitions that the Cross model cannot

Τε Γ [-273]	mperature	Shear rate	Pressure	Viscosity Pars I0:1	-
	10.120.00]	1/3 [0.]		1 0 3 [0.]	
3					
5					-
E	dit test infor	mation			
	Γ	ОК	Cancel	Hel	p

plastics made perfect





Improved Warpage Accuracy for Fiber filled LCP's

- New Micromechanics model: Mori-Tanaka
 - Targeted to improve fiber filled LCP materials by allowing anisotropic mechanical properties for the LCP matrix to be used
 - Influence on warpage results using:
 - Isotropic matrix \rightarrow identical to Tandon-Weng
 - Slightly anisotropic matrix \rightarrow very minor advantage over Tando-Weng

Matrix properties		?		
 Mechanical properties data Elastic modulus, 1st principal direction (E1) 	11000	MPa (0:3e+006)	Composite Property Calculation O	ptions ? 🔀
Elastic modulus, 2nd principal direction (E2) Poissons ratio (v12)	1900 0.44	MPa (0:3e+006) [(0:1)	Closure approximation model Fiber-filled property output	Orthotropic 3
Poissons ratio (v23) Shear modulus (G12)	0.22 3829	(0:1) MPa (0:3e+006)	Micro-mechanics model	Tandon-Weng
Matrix coefficient of thermal expansion (CTE) data – Alpha1 Alpha2	1.3e-006 8.5e-005	1/C (-0.0001:0.03) 1/C (-0.0001:0.03)	Thermal expansion coefficient model	Halpin-Tsai Tandon-Weng Krenchel
		Edit test information	ΠΚ	Cox Ogorkiewicz-WeidmannCounto Mori-Tanaka
	OK	Cancel Help		









Crystallisation and Shear: Eltex PHV 252

 $Tc = 140^{\circ}C$ / without shear :





 $t = 120 \min$





t = 240 min

t = 0

 $t = 60 \min$

Tc = 140° C / γ = 0.5 s⁻¹ / ts = 10s :



t = 0

 $t = 60 \min$

Tc = 140° C / γ = 5 s⁻¹ / ts = 10s :



 $t = 120 \min$



t = 180 min



Crystallisation

- Shear
 - Affects nucleation
 - Decreases crystallisation time

Eder, Janeschitz Kriegl, Lidauer, Prog. Polymer Sci. 1990

 High shear for short time more effective than low shear for longer time

Vleeshouwers and Meijer - Rheol. Acta. 1996

- Shearing for longer periods affects morphology
 - Crystallisation time unchanged
 - Formation of row nuclei

Kumaraswamy et. al. - Macromolecules 1999. Acierno et. al. - Rheol. Acta. 2003. Koscher and Fulchiron, Polymer, 2003.



Effect of FIC on Viscosity



For rough particles A ~0.44 Tanner - JNNFM 2002


Crystallisation & Conductivity

Slab model

$$\mathbf{k}^{-1} = (1 - \alpha) \mathbf{k}_{a}^{-1} + \alpha \mathbf{k}_{s}^{-1}$$

a: amorphous phase

s: solid (semi-crystalline) phase α: relative crystallinity







Specific Heat & Cystallisation

Depends on Cooling Rate



Link to crystallisation

 $c_{p}(\alpha,T) = \alpha c_{p}(T) + (1-\alpha) c_{p}(T)$



Density & Crystallisation

- PVT measured under "static" conditions
- Modify with crystallisation
 - Flow induced
 - Temperature and rate of temperature change

$$v = \alpha v_s + (1 - \alpha) v_a$$



Crystallisation Model

Kolmorgoroff

$$\alpha_{f} = C_{m} \int_{0}^{t} \dot{N}(s) \left[\int_{s}^{t} G(u) du \right]^{m} ds$$
$$\alpha = 1 - exp(-\alpha_{f})$$

- Accounts for affect of
 - Temperature
 - Rate of temperature change
 - Flow induced crystallisation



Pressure Predictions

✓ PP (thickness=3.0mm) 95 Parameters used Hold Pressure = 28.3 MPa 85 ∆H = 92000 J.kg⁻¹.K⁻¹ D3 = 3e-007 75 $\lambda = 2.7$ 65 a_N = 0.156 & b_N = 15.1 Pressure [MPa] HTC = 5000 W.m⁻².K⁻¹ 55 - R&D Progam N99 45 35 - Experiment 25 *** 15 5 -5 0 2 6 10 12 4 Time [s] ⁸ 14

New Results



Young's Modulus (1mm part)





Structural Analysis (FEA)

- Interface to:
 - Abaqus
 - Ansys
 - Patran
 - Nastran
 - -LS-Dyna



Exclusive structural analysis for optimising the structural integrity of plastic injection moulded parts.



Information Exported from Moldflow to FEA

- Unfilled Materials

- Elastic modulus, Shear modulus & Poisson's ratio from Material database
- Coefficient of thermal expansion (CTE) from Material database
- Layer-wise (20 layers through the thickness of each element) Residual stresses
- Fiber-filled Materials
 - Layer-wise Elastic modulus, Shear modulus & Poisson's ratio
 - Layer-wise CTE
 - Layer-wise Residual stresses
 - Layer-wise Fiber orientation angle







Microcellular (MuCell®) Injection Moulding Simulation

- MuCell is a variation of foam molding
- This process is marketed by Trexel Inc.
- In this process a Super Critical Fluid (SCF) of Nitrogen (N₂) or Carbon Dioxide (CO₂) is mixed with polymer melt to create a single phase solution which is then injected into the cavity



The MuCell Process

- **1.** Creation of a single phase solution
- 2. Homogeneous Nucleation
- **3.** Cell Growth
- **4.** Part Formation



The rotating screw draws in the granulate from the material hopper and transports it in the direction of the screw tip.





The plastic is plastified and homogenised by heating while being transported.



The plastics-gas mixture is under pressure and is injected into the injection moulding tool, where it forms small, finely distributed gas bubbles.



mage courtesy of Trexel Inc.

Advantages of MuCell

- Lighter parts (due to material reduction)
- Thin and difficult-to-fill sections can now be filled (due to reduction in material viscosity)
- Reduced cycle times
- Reduced pressures
- Reduced clamp tonnage
- Reduced part warpage



MuCell Gas Properties

All MuCell ® material properties (System)		Molecular weight of the gas	44	
Description CO2 N2 N2 N2 N2 N2 N2 N2	Surface tension Viscosity coefficients for gas v1 v2 v3 Solubility coefficients for gas k1 k2	5e-005 1 -17.135 186.95 1.5361e-009 1.9829e+005	N/mm	
	Export	d1 d2	8.741e-008 -2830.5	
		Name CO2	ОК	Help



MuCell User Inputs

Microcellular Injection Molding Settings - Page 2 of 2

Volume filled at start of foaming Initial bubble radius Number of cells per volume Initial gas concentration

90	% [0:100]	
0.001	mm [0:1]	
2e+011	1/m^3 [0:1e+020]	
0.5	% [0:1]	



Simulation Results



Bubble Radius at the end of cycle



Simulation Results



Bubble Radius as a function of time



Bubbles

Three points to be compared: black: near the gate red: middle of the part blue: end of flow

The blue one has a lower pressure and a bigger bubble radius at the wall than the other points.



Simulation Results



Predicted Shape & Magnitude of part deflection





MuCell Validation



Short shot comparison for gas concentration of 0.5% (by weight) and shot size of 70%



Birefringence





What is Birefringence?

- Definition: Birefringence is the change in the refractive index of polarised light passing through an object
- Birefringence may lead to crucial part defects
 - Blurred images
 - Double images
 - Poor optical performance





Birefringence: Polymers

- Birefringence can be caused by stresses in polymer
 - Flow induced stresses
 - Post warpage induced stresses
- Elastic deformation caused by residual stresses
- Viscoelastic deformation caused by flow orientation of polymer
- Will not be uniform in all regions of the part or through the thickness
- Need viscoelastic material data to predict change in optical properties









Stress-optical law

$$\Delta n_{ii} = C_1 \sigma_{ii} + C_2 (\sigma_{11} + \sigma_{22} + \sigma_{33})$$

$$\Delta n_{ij} = C_1 \sigma_{ij} \qquad i \neq j$$

Δn_i	Change in refractive index
σ	Stress
<i>C</i> ₁	Stress-optical coefficient (anisotropic)
<i>C</i> ₂	Stress-optical coefficient (isotropic)

The final residual stresses are determined after ejection.



Generalized Voigt-Kelvin Model

 Complex viscoelastic behaviour can be described by elements with different properties, coupled in series





Testing Viscoelasticity - Methods

- Dynamic Mechanical Analysis
 - Parallel Plate



Rectangular Torsion





Viscoelastic data - Parallel Plate

 The elastic modulus (G'), viscous modulus (G") and Viscosity (eta) can be shifted to form a master curve using the principle of "time-temperature superposition"



Viscoelastic data - Master Curve

• The modulus master curves from the parallel plate and rectangular torsion tests can be combined at the reference temperature to show the transition from melt to rubber to glass.





Temperature Shift

- Shows how the retardation spectrum changes for different temperatures
- May use WLF from the melt viscosity but...
- More accurate to use its own parameters

$$t_{i}(T) = t_{i}(T_{ref}) \exp \frac{-A_{1}(T - T_{ref})}{A_{2} + (T - T_{ref})}$$



Birefringence Simulation- Requirements





Material Properties for Birefringence Analysis

- Optical properties
 - Base refractive index
 - Stress optical coefficients of the material
- Viscoelastic data
 - Relaxational spectrum
 - Parallel plate rheom.
 - Grade specific data recommended
- Moldflow Plastics Labs offers testing services for this data
- 6 mats tested so far

ermoplastics material				?				
Description Recomm	nded Processing	Rheologic	al Properties	Thermal Properties				
PV1 Properties Mechanical Pr	operties	Shrinkage Properties	Filler Properties	Uptical properties				
Refractive index for unoriented material Stress-Optical Coefficients C1 C2 Relaxational spectrum Relaxation time at the reference temperal 1 1.198e-1 2 5.375e-1	1.49 -4.6 0 ure Compliance s 1/Pa 109 1.437e-009 108 2.744e-009	Brewster Brewster						
3 2.412e- 4 0.0001 5 0.00 6 0.22 7 9: 8 43 9 19	006 9.311e-009 182 5.529-008 1.04e-006 79 1.234e-006 79 3.884e-006 8.8 1.869e-005 190 0.0005238	Temperature modeTemperature shift forTref432A117.36A2320.2	el for Optical Calcula the ViscoElastic models K K K	tions ?X				
Temperature effect on viscoelaestic model WLF Model ne Sumipex HT55X : Sumitomo Chemical C	ompany	View Temperature	model for Optical Calculatio	ins				
ОК Нер								



Change in Refractive Index

- Difference in refractive index after warpage
- Used to detect changes in refractive index caused by stresses after deformation


Scaled Refractive Index (Cutting Plane)

- Birefringence when tensors in principle directions vary
- Double image
 - If the change in refractive index tensor has no axis along the direction of the incident light
- Polarisation effect (color bands)
 - If one of the axes of the change in refractive index tensor is parallel to the incident light the polarisation of the light will change.



Retardation

- Difference in horizontally and vertically polarised light expressed in length (nanometers)
 - Max should be well under 25% of light wavelength often less (10%)
- Result based on light direction



Retardation for light coming from +Z direction, nm

= 5000.5

Phase Shift

- Difference in horizontally and vertically polarised light expressed in degrees
 - Max should be well under 360° often 90° or lower is a limit
- Result based on light direction



Retardation Measurement Process #1

- Retardation is measured by the Berek compensation technique
- Retardation is measured at 45 points (9x5 grid) offset from cavity edges
- Identical samples are stacked three or more high for greater accuracy
- Reported results are an average for a single sample









Viscoelastic data

- Viscoelastic data is used for birefringence predictions
- The data allows the simulation of the evolving refractive index during the moulding of optical components
- In the future the use of viscoelastic data is likely to be more widespread



Future Work & Challenges

- Flow of high performance polymers
 - Liquid Crystal polymers
 - Use viscoelastic data to measure response in melt & solid
- Crystallinity effects
- Optical
 - Birefringence
 - Surface finish
- Strength
 - Performance under load
- Impact resistance
- Electrical
- Effect of colour on shrinkage
- Rapid cooling PVT data
- PVT for Reactive materials

