

Numerical simulation of the flow of thermosetting plastics: application to injection moulding

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ABSTRACT

An evaluation of a numerical model for simulating the flow of thermosetting plastics, developed at the National Physical Laboratory, is described. The sensitivity of calculations to input data has been assessed, and predictions have been compared with experimental results obtained during production using an injection moulding machine. It has been demonstrated that calculations of mould filling conditions are particularly sensitive to the rheological properties input data, but not to the thermal and physical properties data and processing conditions. The high sensitivity to the rheological data is primarily due to the need to extrapolate the shear viscosity data to the conditions prevalent in injection moulding, namely the conditions of high shear rate and high temperature near the mould wall. The agreement between predicted and measured fill pressures in injection moulding was reasonable considering the magnitude of the potential sources of error identified.

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1 INTRODUCTION

Unsaturated polyester moulding compounds are glass-fibre reinforced thermosetting plastics which are widely used in the manufacture of electrical and domestic appliances and in the transportation industry (1-7). Unsaturated polyester materials, in the form of dough moulding compounds (DMCs), are largely processed by injection moulding, resulting in considerable financial benefits and greater technical complexity of finished articles over the more traditional processing route of compression moulding (1). The mechanical properties of mouldings, determined by their microstructure, are influenced by the rheological behaviour of the plastics and by the processing conditions employed (8-11). An understanding of, and an ability to predict reliably the flow behaviour of DMCs will therefore lead to the production of improved mouldings, obtained more efficiently and economically through advances in processing, mould design and materials specification. The benefits of being able to model the flow process have been presented more fully in references 12-15.

The broad objective of this study is to obtain an improved understanding of the modelling of flow of thermosetting plastics under injection moulding processing conditions. To achieve this the more specific objectives set were:

- to develop a non-isothermal model for simulating flow in axisymmetric and rectangular geometries;

- to evaluate the model by comparison with measurements made of non-isothermal flows in a simple geometry test case;

- to model the flow occurring in injection moulding of a test geometry and compare calculations with measurements made on an injection moulding machine;

- to assess the sensitivity of calculations of injection moulding fill pressures to the accuracy of the specification of the processing conditions and the material's rheological, thermal and physical properties data;

- to estimate the contribution of extensional flow to the injection moulding fill pressure for the test mould geometry.

The reason for carrying out this work was primarily because there was a dearth of work on, and consequently a lack of understanding of, the modelling of flow of thermosetting plastics in injection moulding. The processing of thermosetting plastics differs fundamentally from that of thermoplastics in that 'cold' material is injected into a 'hot' mould, rather than 'hot' material into a 'cold' mould as is the case for thermoplastics.

A review of the literature indicated that the majority of work undertaken on numerical modelling of flow of plastics was for application to thermoplastics - as was also indicated by Kamal and Ryan (16) and Bowers (17). In their review of the literature Blanc et al (18) commented that no study of the simulation of the mould filling process for unsaturated polyester compounds had been made: the model that was used by these authors was itself initially developed for the simulation of thermoplastics mould filling. Since then, Thomas et al (12) have developed a numerical model for simulating the flow of thermosetting plastics (which was based on a previous model for application to elastomers) and which they reported was undergoing further development.

In this report the finite difference numerical model developed for predicting the flow of thermosetting plastics in simple geometries is described. The predictions of injection mould filling pressures are compared with experimentally measured values obtained using an injection moulding machine. Predictions of isothermal and non-isothermal flows of unsaturated polyester dough moulding compounds (DMCs) in simple geometries and comparisons made with experimental results have been presented elsewhere (19). As a result of this work recommendations for improved practice in both the measurement and modelling of flow of these materials have been made.

2 EXPERIMENTAL DETAILS

2.1 MATERIAL

The material investigated in this work was based upon a model composition of an unsaturated polyester dough moulding compound. The mix, supplied by BIP Chemicals Ltd, had been specially formulated to represent a commercially available grades of DMC, namely a general purpose low-shrink grade and is designated as L7049. The DMC was based on an orthophthalic unsaturated polyester resin and was mineral

filled and glass-fibre reinforced. It contained initiators and inhibitors but no pigmentation. The DMC contained polystyrene, the role of which is to control shrinkage on curing. The glass-fibre reinforcement consisted of individual glass-fibres bound together using a hard size to form bundles of high integrity. These bundles consisted of E-type glass-fibres of diameter 12 μm . The bundles were approximately 0.05 mm thick and up to a maximum of 1 mm in width, and were cut to a nominal length of 6 mm. The composition of the DMC is detailed in Table 2.1. Further details of the material and its rheological characterisation are given in reference 19.

Table 2.1 Composition of DMCs

Component	L7049 (Low-shrink)	
	% wt	% vol
Glass-fibre (6 mm length)	15	12
Mineral filler (including mould release agent)	57	44
Resin + thermoplastic additive	28	44

Figures give percentage by weight (% wt) and by volume (% vol) values.

2.2 MOULDING TRIALS

In Section 3.3 a comparison is made of experimental measurements of injection filling pressures with calculations. To provide the experimental data a modified standard extended nozzle was attached to a Bucher-Guyer 265 tonne injection moulding machine to carry out in-line measurements during the injection moulding of DMCs (19). The nozzle had been fitted with pressure transducers (Kistler Type 601H) to record the injection pressure profile during the moulding cycle. The nozzle temperature was controlled using the injection moulding machine barrel's circulating water temperature control system. Measurements of pressure in the nozzle, flow rate and temperature were made to characterise the moulding cycle to enable comparisons to be made with numerical modelling predictions of mould filling pressures.

The measurements were made whilst injecting into a test mould known as the 'Healey' mould. The 'Healey' moulding produced from this mould cavity is shown, with details

of its approximate dimensions, in Figure 2.1. An example injection pressure versus time trace is presented in Figure 2.2. The fill pressure was taken as the value immediately prior to the rapid increase in pressure marked by 'mould filled' in the Figure. To this value a correction (detailed in reference 19) was made to account for the pressure drop from the transducer position to the end of the nozzle.

3 NUMERICAL MODELLING OF THE FLOW OF DMCs

3.1 DESCRIPTION OF THE FINITE DIFFERENCE MODEL FOR SIMULATING FLOW IN NARROW CHANNELS

A finite difference numerical model for simulating the flow of a fluid in a narrow channel was developed at the National Physical Laboratory. The model was based on that presented by Wijngaarden et al (20). A full description of the model is given by Ferriss (21). A finite difference scheme was used as it was considered to be more suitable than finite element methods for this class of problem, namely that of non-linear flow behaviour in regular geometries. Although the model can also be used for simulating the flow of thermoplastics including solidification effects, the following work will consider only those aspects relevant to the simulation of flow of thermosetting plastics.

The main assumptions of the model are:

- 1 The shear viscosity η is given by a power-law model with the temperature dependence given either by an empirical exponential function or an Arrhenius function

$$\eta = \eta_0 \dot{\gamma}^{n-1} e^{-k\theta}$$

and

$$\eta = \eta'_0 \dot{\gamma}^{n-1} e^{q/\theta}$$

respectively where $\dot{\gamma}$ is the shear rate and η_0 , η'_0 , k and q are constants and θ is the temperature (K).

2. The fluid is incompressible.

3. The heat capacity, density and thermal conductivity of the fluid are constant.
4. The effect of curing on viscosity and exothermic effects are ignored.
5. Fluid inertia terms are ignored.
6. The flow that is considered is that occurring in either a cylindrical channel or a two-dimensional (infinitely wide) slit channel. The channel diameter or thickness is small compared with its length.
7. Axial heat conduction effects are ignored.

The model considered the unsteady flow of the fluid; that is the development with time of the flow from the specified initial conditions to the steady-state flow. However, all of the results presented in this study are for steady-state flow conditions. The boundary conditions specified were the volume flow rate across the inlet, the wall temperature and the fluid inlet temperature. The latter was specified at each individual mesh point across the inlet thus allowing the inlet temperature to be profiled across the section.

In addition to the rheological data given in the appropriate sections below, the following experimentally measured data was also required for modelling the flow of DMCs (22):

specific heat capacity, C_p	=	1175 J/(kg K)
thermal conductivity, κ	=	0.52 J/(s m K)
density, ρ	=	1660 kg/m ³

The mesh used was typically of twelve equi-spaced mesh points in the flow direction and twelve variable-position mesh points in the radial or through-thickness direction located at scaled positions of 0, 0.2, 0.4, 0.6, 0.8, 0.9, 0.95, 0.97, 0.98, 0.99, 0.995 and 1, where 0 defines the position of the centre-line and 1 the channel wall. The difference between the scaled positions of adjacent mesh points defines the thickness of the element between those points. Unless otherwise stated the above conditions have been adopted as standard.

3.2 EVALUATION OF THE NUMERICAL MODEL

General

Validation of the numerical model against analytical isothermal and non-isothermal solutions was reported by Ferriss (21). In modelling the isothermal flow of a power-law fluid using a 12×12 mesh as described in Section 3.1 the ratio of the numerically calculated pressure drop to the analytical solution (23) was 0.983 - ie within 2% of the true value. Also, the numerically calculated centre-line velocity was within 2% of the analytical value. These results indicate that this mesh was suitable for modelling isothermal flows.

Initial modelling work demonstrated that to obtain convergence of the numerical solution the iteration time step had to be proportional to the square of the scaled size of the smallest mesh (scaled as a fraction of the channel dimension). The need for a small wall mesh size for non-isothermal cases (see Section 3.2.2) resulted in many iterative steps being required, and consequently significant computer processing time. Checking that a valid solution had been obtained was carried out by further reducing the iteration time step for the specified problem. If the results were the same then convergence was assumed to have occurred.

Non-isothermal flow

The type of non-isothermal flow that has been considered in this investigation is a simulation of that occurring in the injection moulding of thermosetting plastics, namely the flow of a cold fluid into a hot channel. For such non-isothermal flows it was found that a small mesh size near the wall was required to obtain a reasonably accurate representation of the flow. To illustrate this point the flow of DMC in the sprue of the Healey moulding (Figure 2.1) for a mould filling time of 0.3 s has been examined. This was the shortest fill time that could be achieved in practice for the moulding and thus represents an extreme case. The effect of mesh size nearest the wall on the pressure drop along the sprue channel is presented in Figure 3.1. A decrease in the wall mesh size resulted in an increase in the calculated pressure drop. Results obtained for calculations made using either 12 or 36 axial mesh points indicated a maximum of 4%

difference in pressure drop, this being obtained for the smallest wall mesh size of 0.002. The temperature and velocity profiles at the exit of the sprue are presented in Figure 3.2. These plots show large thermal and velocity gradients near the wall. The flow can be most easily visualised as a low temperature and thus high viscosity core surrounded by a thin, high temperature and thus low viscosity lubricating layer adjacent to the wall.

The shape of the pressure drop versus wall mesh size curves in Figure 3.1 was considered to be due to factors associated with the large thermal gradients and consequently velocity gradients near the wall, Figure 3.2. The velocity profile near the wall could not be accurately described until the mesh size was sufficiently small to resolve changes in the velocity profile. Using a coarser mesh effectively imposed an incorrect velocity profile on the flow. This was a particular problem wherever large thermal gradients existed, for example at the entry to the flow region. The necessary specification of the boundary conditions at the entry plane resulted in the entire difference in the injection and wall temperatures being accommodated over the thickness of the first wall mesh - independent of that mesh's size. The problem was inherently ill-defined as further refinement of the wall mesh would always be accompanied by a change in the definition of the problem. Away from the entry region the thermal and velocity gradients were smaller and mesh size was consequently not so critical. Although the temperatures were ill-defined it is expected that the pressure drop would tend to a steady value with decreasing mesh size. A log-log plot of the pressure drop versus wall mesh size indicates a reduction in the (logarithmic) rate of increase of pressure drop below a wall mesh size of approximately 0.01 for this extreme high flow rate case, Figure 3.3. A wall mesh of 0.005 was adopted as standard - justification for this was as follows. For the sprue this mesh size represents a thickness of 20 μm . To put this dimension into perspective the glass-fibres have a diameter of approximately 12 μm , the chalk particles a diameter of approximately 1 μm , and the surface finish of a DMC moulding measured using a Talysurf had a peak-to-trough roughness of up to approximately 1 μm (24). A further reduction in the mesh size by a factor of ten would have resulted in an increase in the pressure drop by approximately 10% (obtained from a linear extrapolation of Figure 3.3). Similarly, a reduction in the wall mesh thickness to 20 $\text{\AA}$ ($2 \times 10^{-9} \text{ m}$ or approximately 12 carbon atom diameters) would have resulted in a 50% increase in the calculated pressure drop value compared with using the standard 0.005 mesh. The merits of a further significant

reduction in the wall mesh size from 0.005 were considered dubious, for example the fluid could no longer have been justifiably considered a continuum. In addition, a factor of ten reduction in the mesh size would have required a factor of one hundred increase in computer time making calculations prohibitively expensive. For these reasons the 0.005 scaled size wall mesh was adopted.

For the above described extreme high flow rate case the numerical calculations indicated that at the exit of the channel 54% of the velocity change (from a value of zero at the wall) occurred within the first 0.5% of the radial distance from the wall, Figure 3.2. For a 4 mm radius channel this is equivalent to a distance of 0.02 mm from the wall. From the information provided it can be calculated that wall shear rates of approximately 250000 s^{-1} were occurring compared with 13000 s^{-1} had the flow been isothermal. For comparison, a more realistic fill time of 2.45 seconds yielded wall shear rates of approximately 19000 s^{-1} at the exit, compared with 1600 s^{-1} for the isothermal case. On this basis it is clear that high shear rates occur in the injection moulding of thermosetting plastics. It is noted that in processing thermoplastics this high shearing flow effect does not occur as hot material is injected into a cold channel.

Implications of adopting a power-law rheological model

The choice of the rheological constitutive equation will obviously affect the outcome of such modelling work, particularly as these constitutive equations are necessarily used for extrapolation of shear viscosity to both higher and lower shear rates, and also to higher temperatures.

Low shear rates (tending to zero) are found near the centre of symmetric flows such as that occurring in cylindrical and slit channels. As a consequence of the Newtonian plateau generally exhibited by fluids at low shear rates the use of a power-law model will tend to overpredict the shear viscosity at lower shear rates ($< 1 \text{ s}^{-1}$). However, as a consequence of the low shear rates the net effect on energy dissipation (and therefore pressure drop) in the central region is small: energy dissipation in shear flow is proportional to $\sigma \times \dot{\gamma}$ or alternatively $\dot{\gamma}^{n+1}$. The overprediction of viscosity at low rates is therefore of relatively minor importance.

Of greater potential concern is the necessary extrapolation of shear viscosity to higher shear rates. Evidence in the literature for shear viscosities of materials up to shear rates of at least 10^4 s^{-1} indicates that the use of a power-law model might overpredict viscosity values (reference 25 on polyester DMC, 26 on polypropylene PP and 27 on polystyrene PS) or underpredict values (references 28 on PP and 26 on long fibre-filled PP). Only Crowson et al (28) presented a result showing a significant change in the behaviour (increasingly Newtonian) at shear rates greater than 10^5 s^{-1} . The assumption of a power-law model was therefore considered reasonable based on the limited data at high shear rates that was available. However, it was noted in the previous Section that very high shear rates occur near the wall in non-isothermal flows. The extrapolation of data from the relatively low shear rate range of isothermal capillary die rheometry measurements to that needed for modelling is very severe, and consequently the potential for introducing significant errors through this extrapolation process is great.

The extrapolation of viscosity to elevated temperatures is also required in numerical modelling. The temperature dependence of viscosity has been fitted by an empirical exponential model and an Arrhenius model, see Section 3.1. The former gave a slightly better fit to data over the range of temperatures covered in rheological measurements (19). However, in extrapolating the two models to the higher temperatures typical of processing there is a divergence in their behaviour: the empirical model yields the greater temperature dependence. To examine this effect more closely one can consider the extrapolated shear viscosity values based on the optimised values for k and q of $0.0281 \text{ }^\circ\text{C}$ and 2850 K respectively, and assuming identical viscosity values given by the two models at $45 \text{ }^\circ\text{C}$. Compared with the Arrhenius model, the empirical model predicts a shear viscosity value that is 7% less at $70 \text{ }^\circ\text{C}$, 20% less at $100 \text{ }^\circ\text{C}$ and approximately 50% less at the typical processing mould temperature of $150 \text{ }^\circ\text{C}$. Obviously, the choice of the temperature dependence equation is critical for modelling the mould filling process. Capillary extrusion rheometry measurements carried out on a slow-curing DMC at temperatures up to $130 \text{ }^\circ\text{C}$ indicated that the Arrhenius model was preferred (29).

One further complication for extrapolating viscosity values to higher temperatures and shear rates using a power-law model (see Section 3.1) is that the model does not permit the shear rate dependence of viscosity to vary with temperature. Evidence in the

literature indicates that the shear viscosities of fluids at different temperatures tend to converge with increasing shear rate, and this has also been noted to be the case for DMCs (19). The consequence of this for extrapolating to predict shear viscosities at higher shear rates and temperatures is that a power-law model (with coefficients determined for data obtained at low temperatures and shear rates) will underpredict viscosities. The extent of underprediction will tend to increase with the magnitude of the extrapolation.

3.2.4 Effect of variations in the properties of the fluid and in processing conditions on calculations

The effect of small variations in the fluid's properties and in the processing conditions on calculations of pressure drop for flow in the Healey moulding sprue has been examined. Two 'standard' processing conditions were adopted: a high flow rate and a low flow rate condition. These represent the two extremes in flow rate for filling of the Healey mould cavity, Figure 2.1. For each of these flow rates the effects of a small change (either a 10% or a 5 °C increase) in the rheological coefficients η_0 , n and q , specific heat capacity C_p , thermal conductivity κ , density ρ , the injection and wall temperatures and flow rate were investigated.

The standard conditions and the corresponding changes in these conditions are presented in Table 3.1 (page 12). The calculated pressure drop values are also presented therein and have been scaled against the value obtained for the standard conditions case at the same flow rate. The temperature and velocity profiles at the end of the channel for the two standard condition cases are presented in Figure 3.4.

The most significant effects on pressure drop were due to changes in the rheological constants n and q , that is, those used for extrapolating viscosity values to higher shear-rates and temperatures. In comparison the pressure drop was relatively insensitive to variations in the thermal properties and density of the fluid. Increasing the injection temperature or wall temperature reduced the pressure drop due to the higher resultant temperature of the flow.

Of all the parameters investigated in this study the effects of small changes in n and q

on pressure drop were most significantly influenced by flow rate. For the parameter n , examination of the power-law shear stress versus shear rate relationship indicated that a change in the value of n would have a more significant effect at higher shear-rates - as was observed in the numerical results, Table 3.1. Examination of the Arrhenius temperature dependence model indicated that the effect of a 10% increase in q on viscosity at temperatures in the range 120-150 °C should be approximately $\times 1.96$ - 2.07 , and should be independent of flow rate. A factor of $\times 2.03$ was obtained for the low flow rate case which was in agreement with this simple analysis. However, a factor of $\times 1.73$ was obtained for the high flow rate case. An examination of the temperature profile at the exit of the channel, as presented in Figure 3.5, accounts for why the high flow rate factor was smaller at $\times 1.73$. As a consequence of a near doubling in the viscosity of the fluid due to the 10% increase in q , the effect of viscous dissipation heating on the flow became more important. Due to the increased viscous dissipation in the region nearest the wall the temperature in this region increased by more than 10 °C above that of the wall, Figure 3.5. This resulted in a thermal lowering of the viscosity near the wall and thus a reduction in the pressure drop, thereby accounting for why the change in pressure drop for a given change in the value of q was flow rate dependent.

The effects of changes in the other parameters on the calculated pressure drop were little affected by flow rate, Table 3.1. However, the small difference that resulted could similarly be explained in terms of the velocity and temperature profiles and the relative contributions of viscous dissipation and thermal conduction effects.

Table 3.1 Effect of variations in rheological, thermal and processing parameters on numerically calculated pressure drop values.

Parameter	Standard value of parameter	Change in value of parameter	Effect of change on calculated pressure drop - scaled by standard conditions value	
			low flow rate $v = 0.304 \text{ ms}^{-1}$	high flow rate $v = 9.15 \text{ ms}^{-1}$
standard condition	as below	-	1 ($1 \equiv 1.36 \text{ MPa}$)	1 ($1 \equiv 7.07 \text{ MPa}$)
η_o^* - viscosity constant	$1.00 \text{ N s}^n \text{ m}^{-2}$	+ 10%	1.10	1.09
n - shear rate exponent	0.381	+ 10%	1.31	1.43
q - viscosity temperature dependence	2850 K	+ 10%	2.03	1.73
C_p - specific heat capacity	$1175 \text{ J kg}^{-1} \text{ K}^{-1}$	+ 10%	1.01	1.02
κ - thermal conductivity	$0.52 \text{ Js}^{-1} \text{ m}^{-1} \text{ K}^{-1}$	+ 10%	0.99	1.00
ρ - density	1660 kg m^{-3}	+ 10%	1.01	1.02
T_i - injection temperature	45 °C	+ 5 °C	0.98	0.97
T_o - wall temperature	150 °C	+ 5 °C	0.93	0.95
v - mean velocity	0.304 or 9.15 ms^{-1}	+ 10%	1.05	1.04

Notes: $\eta = \eta_o^* \dot{\gamma}^{n-1} e^{q/\theta}$; channel length = 0.14 m, radius = 0.004 m.

3.3 INJECTION MOULDING: COMPARISON OF MEASUREMENTS WITH NUMERICAL CALCULATIONS

Numerical modelling details

In modelling the flow in the Healey mould cavity the wall temperature was taken as 150 °C. The flow into the sprue was modelled using an injection temperature of 45 °C. Other data used were as presented in Tables 3.2 and 3.3. Both the exponential and Arrhenius temperature dependence viscosity models were used in separate analyses. The numerically calculated temperature profile at the outlet of the sprue was then taken to be the temperature profile at the inlet of the runner. The temperature profile at the inlet of the gate (rectangular section) was calculated from the profile at the outlet of the runner (cylindrical section) on the basis of equivalent relative areas - ie the temperature at a scaled radius of x in the runner was the same as at a scaled position of x^2 from the centre-line in the gate where $0 < x < 1$. Thus the same wall, centre-line and average temperatures existed on both sides of the runner-gate interface. Finally, the mould cavity inlet temperature profile was taken to be the same as the gate temperature outlet profile.

The pressure drop in the converging flow region from the runner to the gate was calculated using the Gibson model (30). Further assumptions were made that the runner and gate were of cylindrical cross-section of areas equivalent to that of their true cross-section, and that the convergence angle was 45°. The calculation of the pressure drop using the Gibson model was based on viscosity values at the average temperature of flow at the exit of the runner.

Comparison of experimental results with numerical calculations

Numerically calculated values of the shear flow pressure drop for each section and the average fluid temperature at the end of each section (in brackets) are given in Tables 3.2 (page 15) and 3.3 (page 16) for the exponential and Arrhenius temperature dependence viscosity models respectively. The average end-of-section temperatures calculated using the two models are very similar. The small difference reflects the higher viscosities associated with the Arrhenius model and consequently greater viscous dissipation.

The pressure drop values in the converging flow region calculated using the Gibson model have also been given in Tables 3.2 and 3.3. The values obtained using the two temperature dependence models differed only slightly due to the counteracting effects of the higher end-of-runner average temperature and higher viscosity for the Arrhenius model compared with the exponential model: for example at 70 °C the two temperature dependence models yielded a 5% difference in viscosity, equivalent to the effect on viscosity of a temperature difference of approximately 1.5 °C.

The ratio of the total pressure drop value calculated using the Arrhenius model to that calculated using the exponential model varied from $\times 1.38$ -1.54 for short to long fill times respectively. The calculated pressure drop has been plotted along with the experimentally determined corrected fill pressure drop data in Figures 3.6 and 3.7. From these plots it is clear that the use of the Arrhenius temperature dependence expression gave a better fit to the experimental data than the exponential form. For both models the agreement was better at high flow rates: the Arrhenius model predicted pressure drop values approximately 20% lower for short fill times and 65% lower for long fill times. It is noted that scatter in experimental pressure drop values is of the same order as the observed difference in numerical and experimental pressure drop values. The converging flow pressure drop from the runner to the gate accounted for approximately 25% of the total pressure drop.

The temperature profiles at the start and end of the mould cavity are presented in Figures 3.8 and 3.9. The effect of viscous dissipation can be seen in the temperature profile at the end of the gate (start of the mould cavity) for a fill time of 0.3 s: a temperature approximately 12 °C above that of the wall temperature was reached. These plots show that curing temperatures are reached by a significant amount of the material within the mould cavity, particularly for the long fill time mouldings.

Table 3.2 Calculated pressure drops and end-of-section average temperatures for filling of the Healey moulding, using the exponential form of the viscosity temperature dependence, $e^{-k\theta}$.

Pressure drop, MPa; (End-of-section average temperature, °C)		Injection fill time, s			
		0.3	0.7	2.45	9
Channel section	Sprue	4.66 MPa (50.4 °C)	3.18 (52.2)	1.69 (57.4)	0.85 (67.2)
	Runner	1.68 (51.6)	1.23 (53.7)	0.65 (60.0)	0.32 (71.3)
	Gate	0.39 (52.0)	0.30 (54.2)	0.16 (60.8)	0.08 (72.4)
	Mould cavity	6.95 (69.5)	4.57 (80.1)	2.40 (105.8)	1.19 (139.1)
Total shear flow pressure drop		13.68	9.27	4.90	2.44
Converging flow pressure drop*		7.1	4.7	2.3	1.0
Total pressure drop		20.8	13.9	7.2	3.4

Notes: $\eta = \eta_0 \dot{\gamma}^{n-1} e^{-k\theta}$, $\lambda = \lambda_0 \dot{\epsilon}^{m-1} e^{-k\theta}$
 $\eta_0 = 27700 \text{ N s}^n \text{ m}^{-2}$, $n = 0.381$, $k = 0.0281 \text{ }^\circ\text{C}^{-1}$
 $\lambda_0 = 173000 \text{ N s}^m \text{ m}^{-2}$, $m = 0.43$, $k = 0.0281 \text{ }^\circ\text{C}^{-1}$
 *:- $R_{\text{out}} = 3.75 \times 10^{-3} \text{ m}$, $R_{\text{in}} = 2.52 \times 10^{-3} \text{ m}$, $\alpha = 45^\circ$.

Table 3.3 Calculated pressure drops and end-of-section average temperatures for filling of the Healey moulding, using the Arrhenius form of the viscosity temperature dependence, $e^{q/\theta}$.

Pressure drop, MPa; (End-of-section average temperature, °C)		Injection fill time, s			
		0.3	0.7	2.45	9
Channel section	Sprue	7.07 MPa (51.0 °C)	4.97 (52.7)	2.68 (58.1)	1.36 (67.9)
	Runner	2.66 (52.4)	1.98 (54.7)	1.07 (60.7)	0.54 (71.9)
	Gate	0.63 (53.2)	0.48 (55.3)	0.27 (61.7)	0.14 (73.3)
	Mould cavity	11.40 (71.2)	7.70 (81.0)	4.20 (105.8)	2.20 (138.9)
Total shear flow pressure drop		21.75	15.13	8.21	4.24
Converging flow pressure drop*		7.0	4.6	2.3	1.0
Total pressure drop		28.7	19.7	10.5	5.2

Notes: $\eta = \eta_o \dot{\gamma}^{n-1} e^{q/\theta}$, $\lambda = \lambda_o \dot{\epsilon}^{m-1} e^{q/\theta}$
 $\eta_o = 1.00 \text{ Ns}^n \text{m}^{-2}$, $n = 0.381$, $q = 2850 \text{ K}$
 $\lambda_o = 6.25 \text{ Ns}^m \text{m}^{-2}$, $m = 0.43$, $q = 2850 \text{ K}$
 *:- $R_{out} = 3.75 \times 10^{-3} \text{ m}$, $R_{in} = 2.52 \times 10^{-3} \text{ m}$, $\alpha = 45^\circ$.

4 DISCUSSION

This study of the numerical modelling of flow of thermosetting plastics has demonstrated that it is essential that very small wall meshes are used adjacent to the wall so that the numerics can accurately describe the flow kinematics. This is due to the formation of a hot and therefore low viscosity 'lubricating' layer adjacent to the wall, which consequently gives rise to high velocity gradients (high shear rates) in that region. The presence of the high shearing 'lubricating' layer in the flow of thermosetting plastics is one of the primary fundamental differences between the processing of thermosetting plastics and thermoplastics: it arises in the processing of thermosetting plastics as cold material is injected into a hot channel, but not in the processing of thermoplastics where hot material is injected into a cold channel. For this

reason the author considers that the reliable modelling of flow of thermosetting plastics is more difficult than that of thermoplastics.

Calculations of injection mould filling of the Healey test moulding indicate that the shear rates and temperatures of the process are significantly higher than the range covered by isothermal measurements of viscosity using a capillary rheometer (19). Fluid temperatures of up to approximately 160 °C were calculated for high flow rate, high viscosity cases where viscous dissipation heating effects were significant. Fluid temperatures of the order of 150 °C (the wall temperature) were present in all cases. Very high shear rates developed near the wall of the channel due to a combination of the high flow rate of injection moulding with the hot, low viscosity 'lubricating' layer effect described above. In the shortest injection fill time case, numerically calculated shear rates in the sprue were up to three decades greater than had been obtained in isothermal capillary rheometry measurements.

It is because of the formation of the hot, high-shearing 'lubricating' layer that the calculations of fill pressure are sensitive to the shear viscosity's shear rate and temperature dependence parameters. The shear viscosity parameters which were provided as input data for modelling were based on measurements made with a relatively low maximum shear rate and low maximum temperature compared with the conditions predicted by the modelling. Thus the numerical model necessarily uses the shear viscosity parameters n and q to extrapolate shear viscosity data to the high shear rates and temperatures required: this extrapolation is considerable and is the origin of the great sensitivity of the calculations to these viscosity parameters.

Nevertheless, the numerically calculated Healey moulding fill pressures using the Arrhenius temperature dependence model were in reasonable agreement with experimentally measured values for short fill times, Figure 3.7. For the shortest fill time the numerical model underpredicted the fill pressure value by approximately 20%. However, as fill time increased the discrepancy also increased by up to a value of 65%. This increased discrepancy could be, in part, due to experimental error. In comparison, the use of the exponential model gave fill pressures approximately 45% lower than the Arrhenius model, Figure 3.6 cf Figure 3.7. This would indicate that the use of the Arrhenius model was better for extrapolating to the higher temperatures encountered in such flows.

As described above the evaluation of the numerical model indicated that the calculations were highly sensitive to the shear rate exponent n and the temperature dependence coefficient q . Variations in other rheological, thermal and processing parameters had at most a 1:1 effect on the calculated pressure drop. Errors in the values assigned to these latter parameters was therefore unlikely to be the source of error in the calculated pressure drop values. The 20% discrepancy in calculated and measured fill pressures for the shortest fill time moulding could be accounted for by a 3-5% error in the value of n or q , Table 3.1. However, an error in the value of n would not account for the increased discrepancy in the calculated and experimentally measured fill pressures at lower flow rates. An error in the value of n would have a greater effect on the pressure drop value for the short fill time rather than the longer fill time moulding condition, Table 3.1. An error in the value of q could potentially account for some of the increased discrepancy at longer fill times, based on the argument presented in Section 3.2.4. However, it is considered that on the basis of the evidence presented this effect would not account solely for the magnitude of the variation in the difference of measured and calculated fill pressures with flow rate.

Additional possible explanations for the greater difference in measured and calculated fill pressures at lower flow rates are that it could be accounted for by scatter in experimental results and/or by an increase in the viscosity of the material during filling due to curing. Temperatures in excess of the curing temperature were present in the region nearest the wall for all flow rate cases. For longer fill times these high temperatures were sustained for longer periods of time, and would be more likely to have an effect on the viscosity of the DMC. This would result in the longer fill time mouldings needing a relatively higher fill pressure than had curing not occurred, thereby accounting for the increased discrepancy in calculated and measured pressure drop values. Blanc et al (18) in their study of mould filling concluded that an increase in pressure at low flow rates or high temperatures occurred as a result of crosslinking. If significant curing of these cure-inhibited materials occurred during mould filling then the effects of the reaction exotherm on temperature, and consequently on pressure drop might also have to be considered. Work on modelling of the inhibition and curing behaviour of these materials and their effect on rheological behaviour is reported elsewhere (31, 32).

Furthermore the effect of the pressure dependence of viscosity has not been taken into consideration in these calculations, and might also partially account for the lower calculated fill pressures compared with the experimentally measured values. Also this work has highlighted the importance of accurately modelling the plastics layer nearest the channel wall as this thin layer dominates the overall flow behaviour. The assumptions made in modelling were that the wall was a perfect thermal conductor at constant temperature and that the thermosetting plastics was in perfect thermal contact with the wall. Considering the importance of the wall layer on the flow behaviour, the effect of making these assumptions should be examined further.

The use of the Gibson model (30) to estimate the pressure drop in the converging flow region from the runner to the gate of the Healey moulding indicated that this pressure drop was approximately 25% of the total pressure drop. The uncertainties in this value were large due to the assumptions made in the analysis. Nevertheless, this was a significant contribution to the total pressure drop and suggests that such extensional flow pressure drop components cannot be ignored if accurate modelling of the flow is required.

In the light of these comments the extent of the agreement that had been obtained between the calculated and experimental values of the injection moulding fill pressure is considered to be quite reasonable.

5 CONCLUSIONS

The following major conclusions are drawn from this work:

Calculations of the injection moulding fill pressure drop for a test moulding were in reasonable agreement with experimentally measured values but were in all cases lower.

To accurately model the injection moulding of thermosetting plastics small mesh sizes are needed adjacent to the wall due to the formation of a hot, high-shearing layer in that region.

The calculation of the shear flow component of the pressure drop was particularly sensitive to the values used for the shear viscosity's shear rate and temperature dependence coefficients, and also to the form of the equation used to describe the temperature dependence of viscosity.

Calculations were comparatively insensitive to other relevant physical properties of the material; namely the thermal conductivity, specific heat capacity, the shear viscosity pre-exponent η_0 and density.

The effect of variations in the processing conditions on the calculated fill pressure drop was small.

The pressure drop in the converging flow region from the runner through the gate (estimated using the Gibson model) was a significant part of the total pressure drop, indicating that this extensional flow component should not be ignored in modelling injection moulding flows of such materials.

Improvement in the accuracy of modelling of flow of thermosetting plastics could be achieved by improving the accuracy of the process of extrapolating shear viscosity values to higher shear rates and temperatures through the use of improved constitutive equations, and by increasing the upper limits of shear rate and temperature at which viscosity measurements are made.

In summary, this work has identified the complications faced in modelling the flow of thermosetting plastics in conditions typical of injection moulding processing. In particular, it has identified the importance of the need for accurate viscosity data at the high shear rates and temperatures found in injection moulding. The lack of this data is the primary limiting factor in being able to accurately model the flow in injection moulding of thermosetting plastics.

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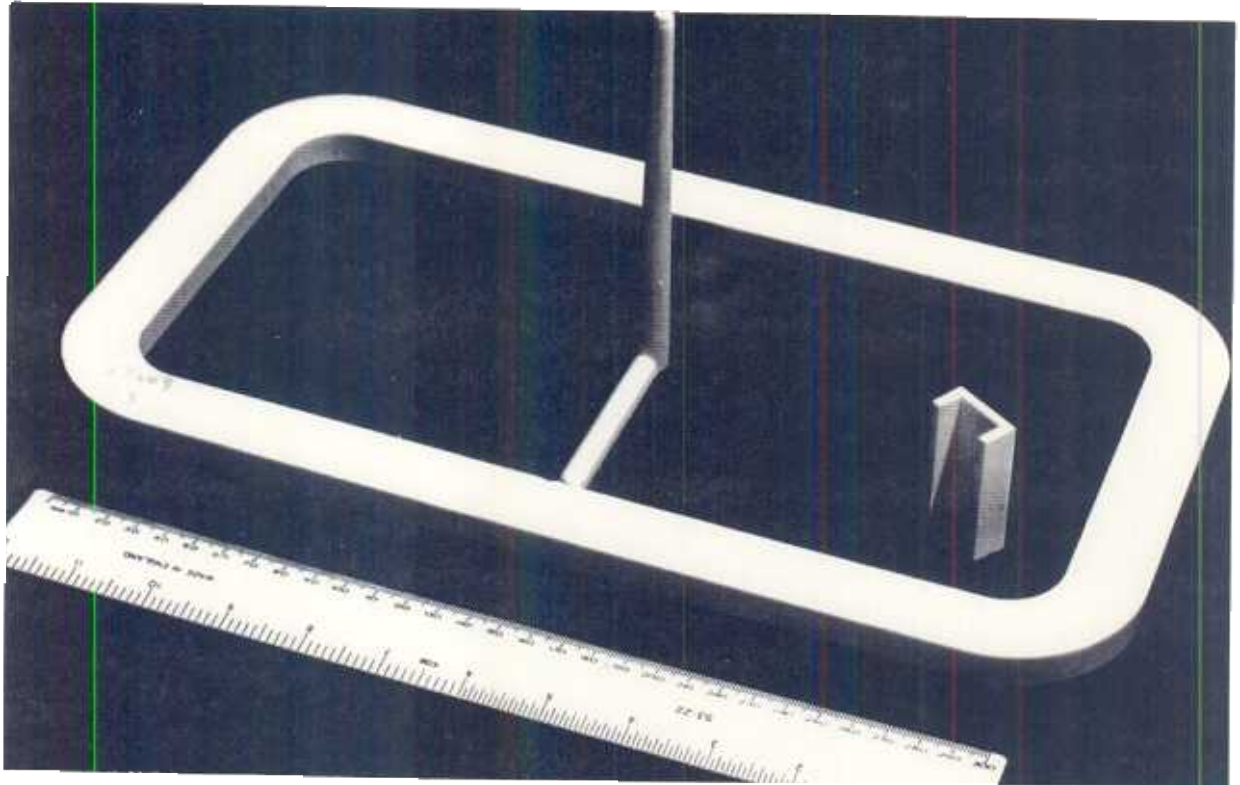
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Approximated moulding geometry and dimensions

Sprue:	cylindrical channel of diameter 8 mm and length 140 mm
Runner:	cylindrical channel of diameter 7.5 mm and length 63 mm
Gate:	rectangular channel of width 10 mm, thickness 2 mm and length 5 mm
Mould cavity:	rectangular channel of width 43 mm, thickness 3.1 mm and length 480 mm

Figure 2.1 'Healey' test moulding

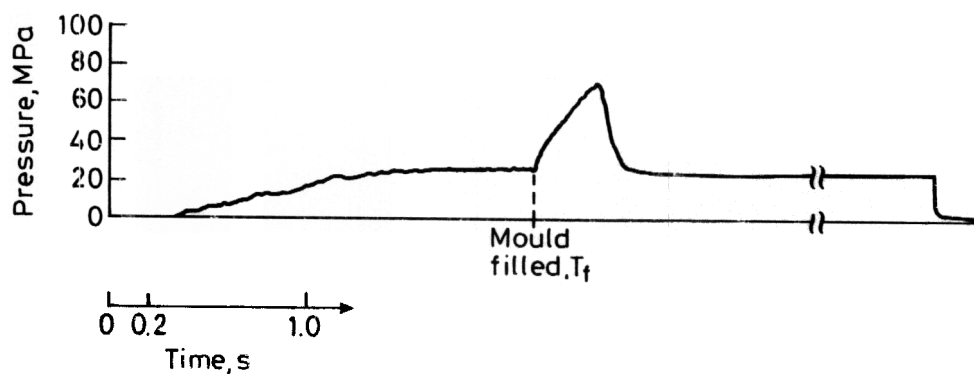
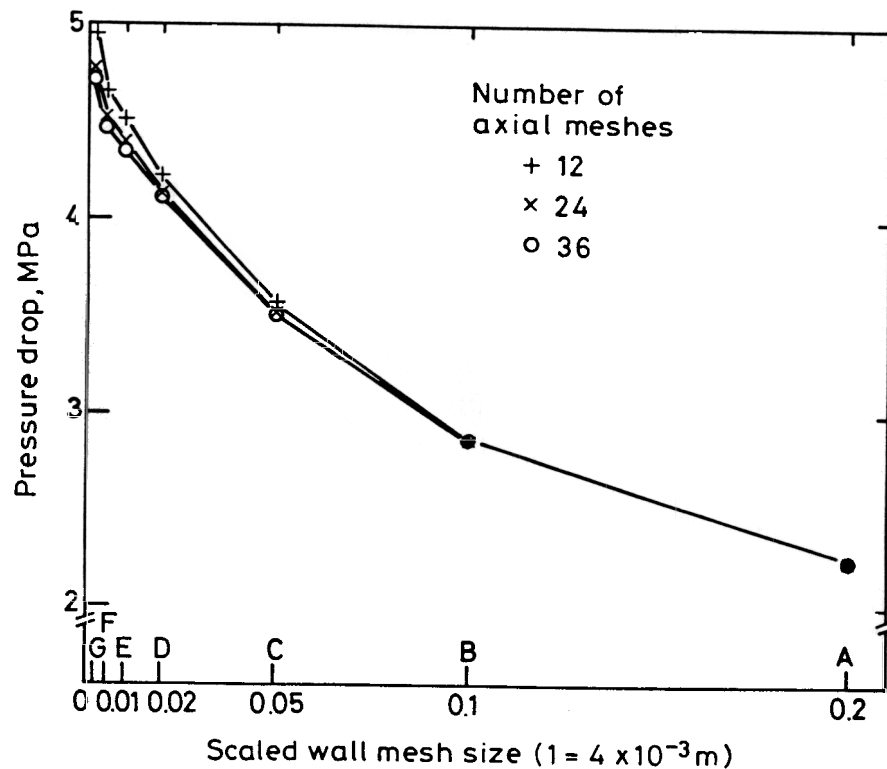


Figure 2.2 Example of injection moulding pressure trace obtained whilst moulding a Healey moulding.



Flow specification:- flow rate $Q = 0.46 \times 10^{-3} \text{ m}^3\text{s}^{-1}$;
 $\eta = \eta_0 \dot{\gamma}^{n-1} e^{-k\theta}$ where $\eta_0 = 2.77 \times 10^4 \text{ N s}^n\text{m}^{-2}$,
 $n = 0.381$, $k = 0.0281 \text{ }^\circ\text{C}^{-1}$;
 wall temperature = $150 \text{ }^\circ\text{C}$; fluid temperature at inlet = $45 \text{ }^\circ\text{C}$;
 channel radius = $4 \times 10^{-3} \text{ m}$, length = 0.14 m .

Mesh specification:

Mesh spec.	Scaled mesh size						
	0.2	0.1	0.05	0.02	0.01	0.005	0.002
A	5	-	-	-	-	-	-
B	4	2	-	-	-	-	-
C	4	1	2	-	-	-	-
D	4	1	0	5	-	-	-
E	4	1	1	1	3	-	-
F	4	1	1	1	2	2	-
G	4	1	1	1	1	2	5

(Note: smallest mesh is the wall mesh)

Figure 3.1 Effect of wall mesh size on calculated pressure drop, simulating flow in the sprue of the Healey moulding (see Figure 2.1).

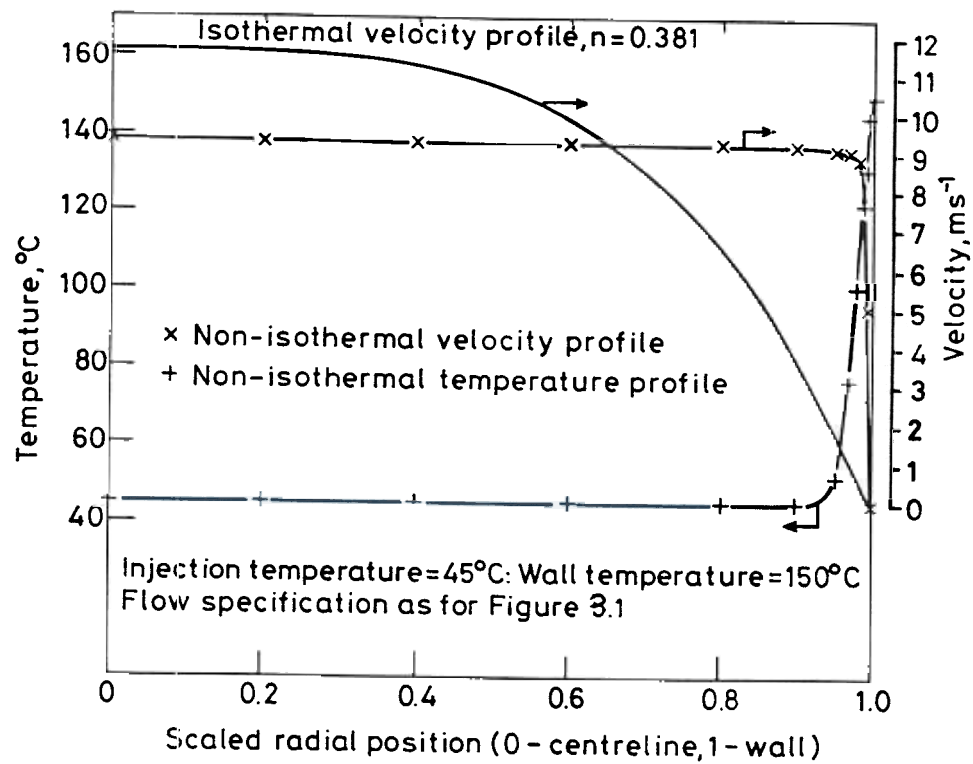


Figure 3.2 Temperature and velocity profile at the exit of the channel.

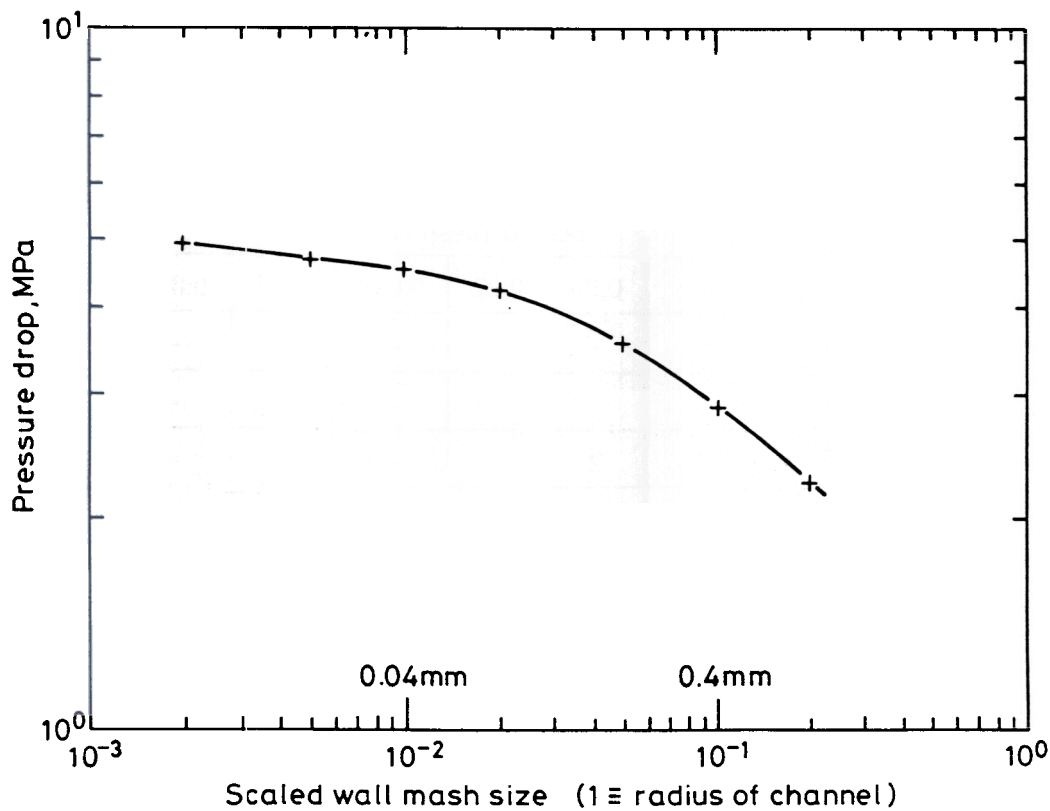


Figure 3.3 Effect of wall mesh size on calculated pressure drop, simulating flow in a sprue. Legend as for Figure 3.1.

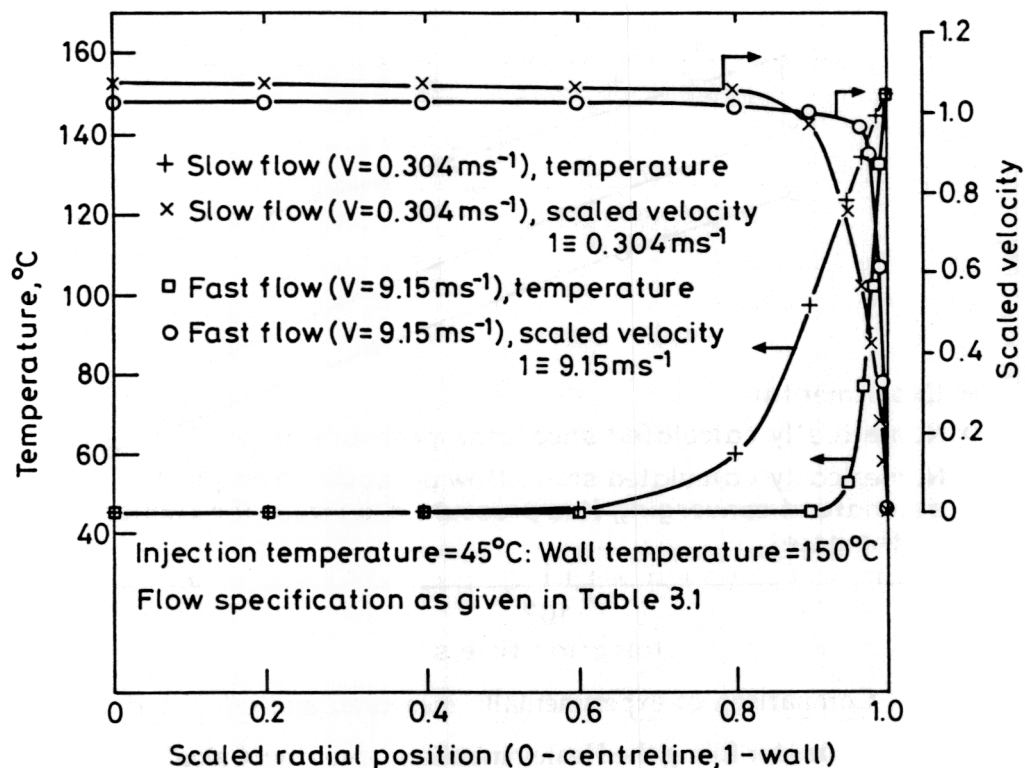


Figure 3.4 Temperature and velocity profiles at end of the channel for high and low flow rates.

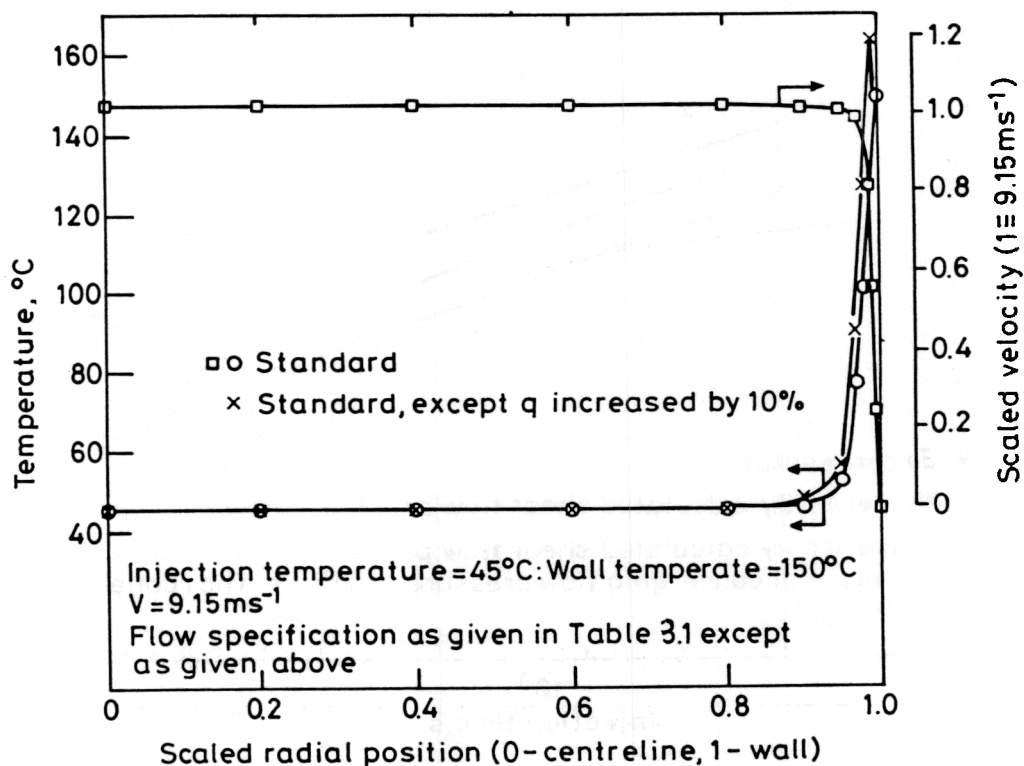


Figure 3.5 Effect of an increase in q on the temperature profile at the exit of the channel illustrating the viscous dissipation heating effect near the wall.

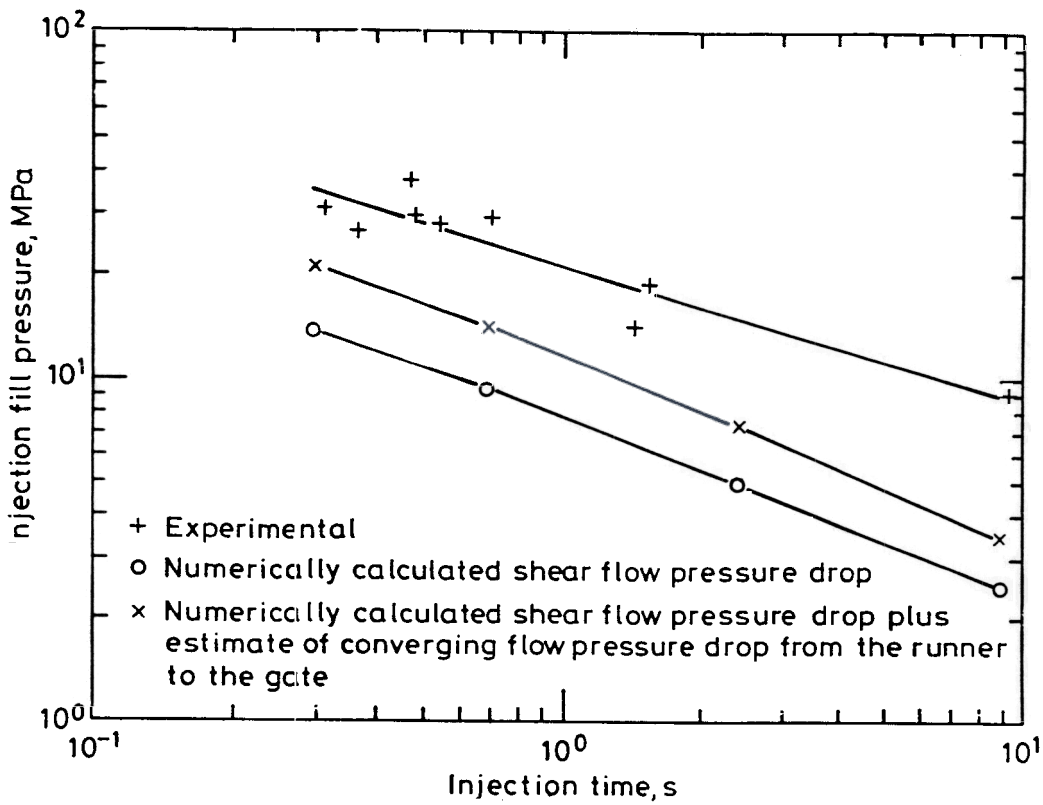


Figure 3.6 Comparison of experimentally measured and calculated pressure drop values for filling the Healey injection moulding. Calculations made using the exponential form of viscosity temperature dependence $e^{-k\theta}$.

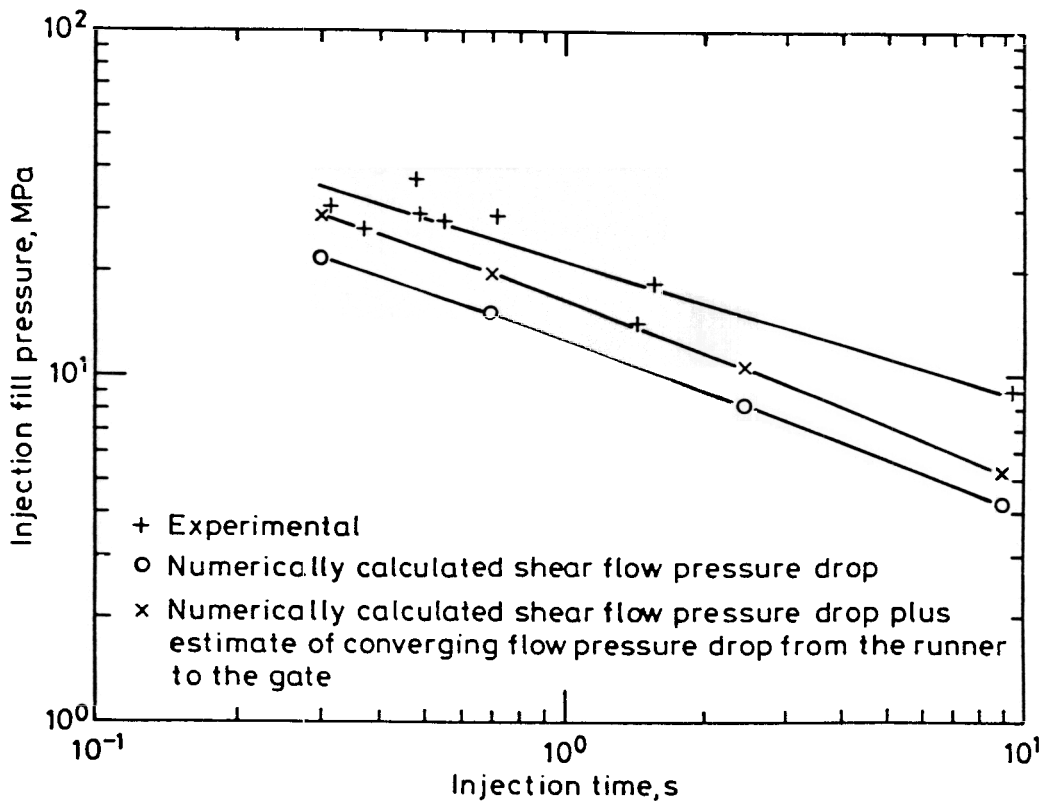


Figure 3.7 Comparison of experimentally measured and calculated pressure drop values for filling the Healey injection moulding. Calculations made using the Arrhenius form of viscosity temperature dependence, $e^{q/\theta}$.

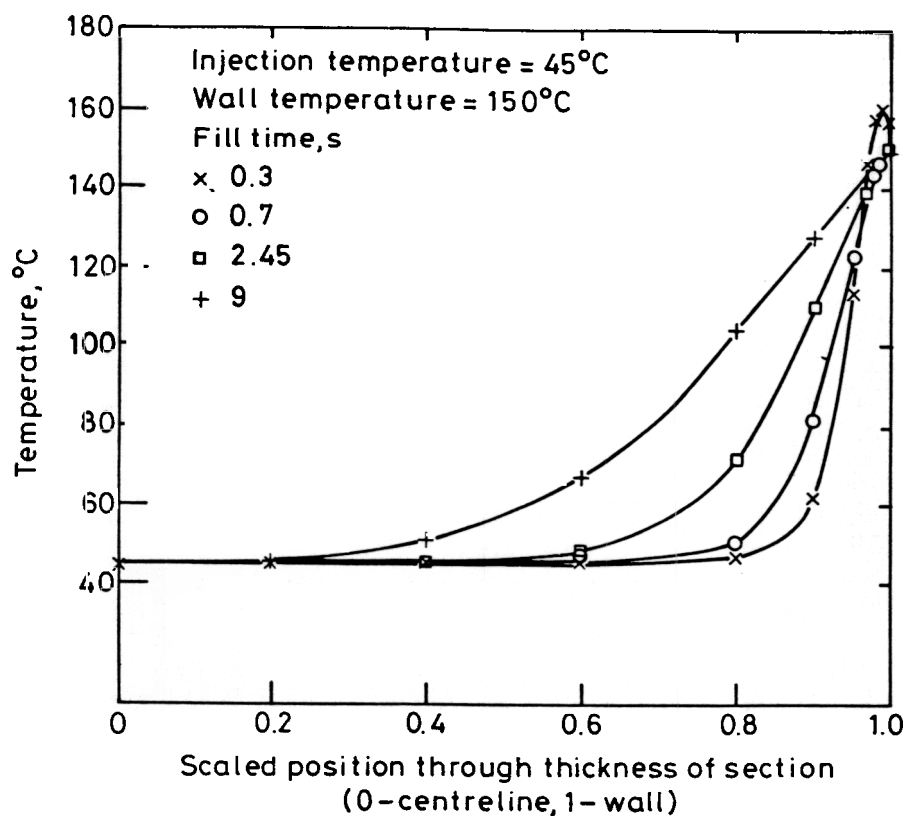


Figure 3.8 Temperature profile at the entrance of the Healey mould cavity for various fill times. Arrhenius model, $e^{q/\theta}$.

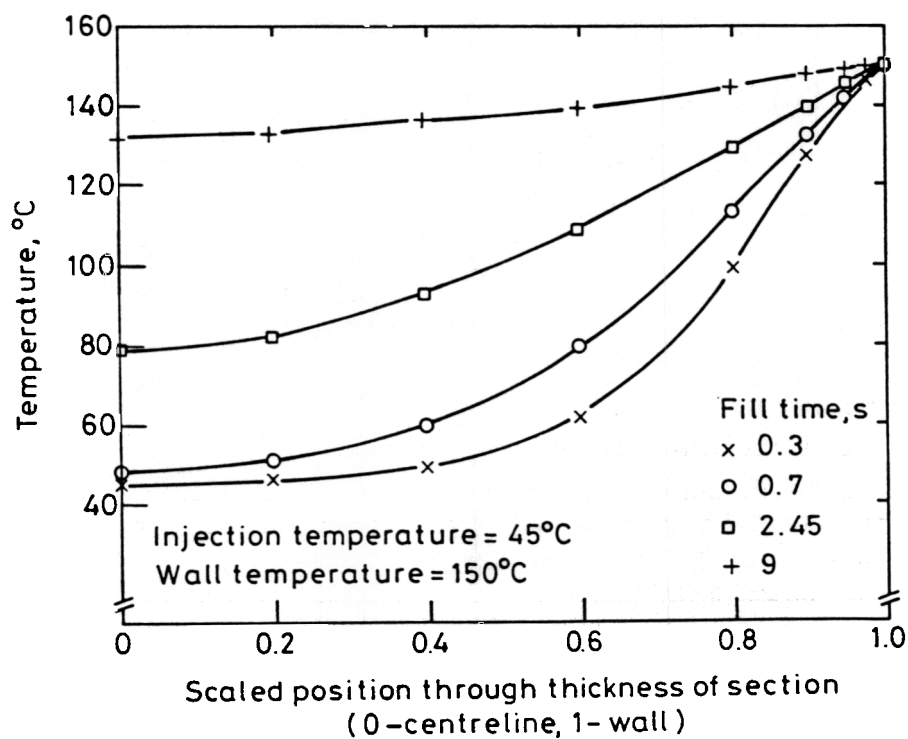


Figure 3.9 Temperature profile at the end of the Healey mould cavity for various fill times. Arrhenius model, $e^{q/\theta}$.