

Temperature equation for compressible polymeric fluids



Amr Guaily

Engineering Math and Physics Department, Faculty of Engineering, Cairo University, Giza 12613, Egypt

ARTICLE INFO

Article history:

Received 28 April 2015

Received in revised form

8 September 2015

Accepted 21 September 2015

Available online 25 September 2015

Keywords:

Polymeric fluids

Temperature equation

Compressibility and elasticity

ABSTRACT

A temperature equation accounting for the compressibility as well as the elasticity of polymeric fluids is derived using the Massieu thermodynamic potential. The constitutive model is completed by adopting the Tait equation relating the thermodynamic pressure to the specific volume and the temperature. A Lagrangian numerical technique is used to study the behavior of the proposed model under different types of loading conditions against published models with an apparent degree of success.

© 2015 Elsevier Ltd. All rights reserved.

1. Introduction

Compressibility effects is of a major importance in that many polymer processes involve rapid cooling to a final, typically non-equilibrium, glassy state [1]. Several theories have been developed to account for polymer non-isothermality taking into account the fluid compressibility and/or elasticity. One of these theories is the theory of purely entropic elasticity developed by Astarita and co-workers ([2–5]) but it does not receive wide acceptance since it does not account for the fluid elasticity [6] nor compressibility. This theory assumes the internal energy to be a function of the temperature only which means that all the mechanical energy is dissipated as heat. The other extreme is the theory of purely energetic elasticity in which all the mechanical energy is stored and could be retrieved. Viscoelastic materials behave intermediately between that of entropy elasticity and energy elasticity [7]. Other models based on non-equilibrium thermodynamics are proposed by Wapperom and Hulsen [8] and Grmela et al. [9] accounting for both compressibility as well as elasticity of the material. The most visible difference between the analysis of Grmela et al. [9] and of Wapperom and Hulsen [8] is in the choice of the state variables and in the entropy balance [10]. It is worth mentioning that the isothermality assumption is not generally accepted for compressible flows since compressible flows are accompanied, in most cases, by considerable temperature variations as noticed experimentally by Flaman and Veltman [11]. The challenge posed by Flaman and

Veltman [11] to numerical simulations to capture the two experimentally-observed phenomena namely, the temperature rise due to sudden increase in the pressure by few hundred Bars and the time delay in measuring the pressure during the injection molding, could only be met by considering the fluid compressibility as well as non-isothermality. The aim of the current work is to present a temperature equation for polymeric fluids taking into account the fluid compressibility as well as elasticity.

2. The compressible temperature equation

To overcome the main drawback of the theory proposed by Astarita and co-workers ([2–5]) namely assuming the internal energy as a function of the temperature only, it is assumed for a compressible viscoelastic material in the presence of thermal effects, the internal energy to be a function of the density, temperature and the conformation tensor [12]. Compressibility effects is represented by adding the density as a new argument while the elasticity effects is captured by considering the conformation tensor as a one more argument. The conformation tensor is considered since it became of great importance for the current modeling of constitutive equations ([12–16]).

Assuming the internal energy as a function of the density, the temperature and conformation tensor as:

$$e = e(\rho, T, \mathbf{c}) \quad (1)$$

where e is the internal energy per unit mass, ρ is the density, T the temperature, and \mathbf{c} is the conformation tensor.

E-mail address: a.guaily@eng.cu.edu.eg.

To get an evolution equation for the temperature, one could write:

$$\frac{De}{Dt} = \frac{\partial e}{\partial T} \Big|_{\rho, \mathbf{c}} \frac{DT}{Dt} + \frac{\partial e}{\partial \rho} \Big|_{T, \mathbf{c}} \frac{D\rho}{Dt} + \frac{\partial e}{\partial \mathbf{c}} \Big|_{\rho, T} : \frac{D\mathbf{c}}{Dt} \quad (2)$$

where t denotes time, $D(\cdot)/Dt$ is the material time derivative, and $(:)$ is the double-contraction operation.

Recall the energy equation for non-polar continuum with no heat sources is;

$$\rho \frac{De}{Dt} = \boldsymbol{\sigma} : \mathbf{d} - \nabla \cdot \mathbf{h} \quad (3)$$

where $\boldsymbol{\sigma}$ is the Cauchy stress tensor, \mathbf{h} is the heat flux vector, and \mathbf{d} is the symmetric part of the velocity gradient defined as:

$$\mathbf{d} = \frac{1}{2} (\nabla \mathbf{v} + (\nabla \mathbf{v})^T) \quad (4)$$

where \mathbf{v} is the velocity vector. Using (3) into (2), one reaches:

$$\rho \frac{\partial e}{\partial T} \Big|_{\rho, \mathbf{c}} \frac{DT}{Dt} + \rho \frac{\partial e}{\partial \rho} \Big|_{T, \mathbf{c}} \frac{D\rho}{Dt} + \rho \frac{\partial e}{\partial \mathbf{c}} \Big|_{\rho, T} : \frac{D\mathbf{c}}{Dt} = \boldsymbol{\sigma} : \mathbf{d} - \nabla \cdot \mathbf{h} \quad (5)$$

For a simple (i.e. one component) polymeric fluids the thermodynamic potential can be split into two contributions ([13–16]):

$$\omega(\rho, T, \mathbf{c}) = \omega_L(\rho, T) + \omega_e(\rho, T, \mathbf{c}) \quad (6)$$

where $\omega(\rho, T, \mathbf{c})$ is the Massieu function and is selected to be the thermodynamic potential since it depends on the same arguments assumed for the internal energy [12]. $\omega_L(\rho, T)$ is the liquid contribution due to intermolecular interactions and $\omega_e(\rho, T, \mathbf{c})$ is the elastic contribution due to the internal microstructure. The Massieu function is defined as [16]:

$$\omega(\rho, T, \mathbf{c}) = s - \hat{e} \frac{\partial s}{\partial \hat{e}} \quad (7)$$

where s is the specific entropy and \hat{e} is the specific internal energy per unit volume defined as:

$$\hat{e} = T^2 \frac{\partial \omega}{\partial T} \quad (8)$$

The liquid contribution to the thermodynamic potential is taken to be Spencer-Gilmore Potential [12]:

$$\omega_L(\rho, T) = \rho \alpha k_B \left\{ 1 + \ln \left[\left(\frac{1}{\rho \alpha} - \frac{1}{\rho_0 \alpha} \right) v T^{3/2} \right] \right\} - \frac{\pi}{T} \quad (9)$$

which is the thermodynamic potential of a van-der-Waals fluid, k_B is the Boltzmann constant and α^{-1} is the mass of a single atom or molecule and can be calculated as $\alpha = N_A/M_W$, with N_A is the Avogadro's number and M_W is the molecular weight of interacting units in the fluid. ρ_0 , π , v are material constants.

Assuming the polymeric fluid to obey the Hookean dumbbell model; the elastic part of the Massieu function could be written as [12]:

$$\omega_e(\rho, T, \mathbf{c}) = \frac{\alpha \rho}{2} \left[k_B \ln(\det \mathbf{c}) - \frac{k(T)}{T} \text{tr} \mathbf{c} \right] \quad (10)$$

where $\text{tr} \mathbf{c}$ and $\det \mathbf{c}$ denote the trace and the determinant of the conformation tensor, respectively and $k(T)$ is the temperature-dependant spring constant.

This form for the elastic contribution doesn't vanish at equilibrium, to correct this flaw; we suggest the following simple modification:

$$\omega_e^m(\rho, T, \mathbf{c}) = \frac{\alpha \rho}{2} \left[k_B \ln \left(\frac{\det \mathbf{c}}{\det \mathbf{c}_0} \right) - \frac{k(T)}{T} (\text{tr} \mathbf{c} - \text{tr} \mathbf{c}_0) \right] \quad (11)$$

where $\text{tr} \mathbf{c}_0$ and $\det \mathbf{c}_0$ are the temperature-dependant trace and the determinant of the conformation tensor, respectively at equilibrium.

Using (9) and (11) into (8); the specific internal energy for compressible viscoelastic fluid is:

$$\hat{e}(\rho, T, \mathbf{c}) = \pi + \frac{3}{2} \rho R_p T + \frac{\alpha \rho}{2} \left(k(T) - T \frac{dk(T)}{dT} \right) (\text{tr} \mathbf{c} - \text{tr} \mathbf{c}_0) \quad (12)$$

where $R_p = \alpha k_B$ is a specific polymer constant with units $\text{J kg}^{-1} \text{K}^{-1}$. Then the specific internal energy per unit mass is $e = \hat{e}/\rho$:

$$e(\rho, T, \mathbf{c}) = \frac{\pi}{\rho} + \frac{3}{2} R_p T + \frac{1}{2} \alpha \left(k(T) - T \frac{dk(T)}{dT} \right) (\text{tr} \mathbf{c} - \text{tr} \mathbf{c}_0) \quad (13)$$

Using the temperature-dependant spring constant defined by Gupta and Metzner [17]:

$$k(T) = f(T) k_B T \quad (14)$$

the function $f(T)$ is given by the empirical relationship:

$$f(T) = \nu T^{-(B+1)} \quad (15)$$

with $B < -1$ and ν is a positive constant. Using the definition of the spring constant, one reaches:

$$e(\rho, T, \mathbf{c}) = \frac{\pi}{\rho} + \frac{3}{2} R_p T - \frac{1}{2} R_p T^2 \frac{df(T)}{dT} (\text{tr} \mathbf{c} - \text{tr} \mathbf{c}_0) \quad (16)$$

Equation (16) represents the specific internal energy for a compressible viscoelastic material and hence could be used to evaluate the partial derivatives needed in Equation (5).

Define c_v as the specific heat at constant volume and conformation tensor as:

$$c_{V, \mathbf{c}} = \frac{\partial e}{\partial T} \Big|_{\rho, \mathbf{c}} = \frac{3}{2} R_p - TR_p \left(\frac{df(T)}{dT} + \frac{T}{2} \frac{d^2 f(T)}{dT^2} \right) (\text{tr} \mathbf{c} - \text{tr} \mathbf{c}_0) \quad (17)$$

which shows that; around equilibrium, the value for the specific heat at constant volume and conformation tensor reduces to the liquid contribution, namely, $1.5R_p$. For the second term of the right hand side of Equation (5), using the definition of the internal energy (16), one reaches:

$$\rho \frac{\partial e}{\partial \rho} \Big|_{T, \mathbf{c}} \frac{D\rho}{Dt} = \pi \text{tr}(\mathbf{d}) \quad (18)$$

The third term of the right hand side of Equation (5) simplifies to:

$$\rho \frac{\partial e}{\partial \mathbf{c}} \Big|_{\rho, T} : \frac{D\mathbf{c}}{Dt} = -\frac{1}{2} \rho R_p T^2 \frac{df(T)}{dT} \frac{D \text{tr}(\mathbf{c})}{Dt} \quad (19)$$

Then the evolution equation of the temperature is:

$$\rho c_{V, \mathbf{c}} \frac{DT}{Dt} = \tau : \mathbf{d} - \nabla \cdot \mathbf{h} - (p + \pi) \text{tr}(\mathbf{d}) + \frac{1}{2} \rho R_p T^2 \frac{df(T)}{dT} \frac{D \text{tr}(\mathbf{c})}{Dt} \quad (20)$$

In which the Cauchy stress tensor is decomposed as:

$$\boldsymbol{\sigma} = -p\mathbf{I} + \boldsymbol{\tau} \quad (21)$$

where \mathbf{I} is the identity tensor, p is the thermodynamic pressure determined from an appropriate equation of state, to be discussed in the following section. And $\boldsymbol{\tau}$ is the extra-stress tensor that vanishes at equilibrium and consists of two parts:

$$\boldsymbol{\tau} = \boldsymbol{\tau}_s + \boldsymbol{\tau}_p \quad (22)$$

where $\boldsymbol{\tau}_s$ is the solvent contribution and $\boldsymbol{\tau}_p$ is the polymer contribution to be determined from an appropriate constitutive equation for compressible non-isothermal viscoelastic liquids e.g. [16]. In Equation (20); the first term on the right hand side represents the viscous-dissipation effects, the second term represents the compressibility effects while the elasticity effects are accounted for by the last term.

It is important to recall that Equation (20) is derived using the Spencer-Gilmore potential for the liquid contribution to the thermodynamic potential and so, different forms could be derived in the same way using more relevant thermodynamic potential for the material under consideration e.g. the modified Flory-Orwoll-Vrij potential [12]. Without considering the liquid contribution to the thermodynamic potential, Ionescu et al. [6] derived the incompressible version of Equation (20). That is why they have to determine the specific heat experimentally, namely Equation (17). The temperature distribution resulting from the present model by numerical simulation is compared with the distribution resulting from the model proposed by Wapperom and Hulsen [8]. In appendix A, the temperature equation, for a single mode, derived by Wapperom and Hulsen [8] is presented and the relation between the specific heat at constant volume used in the present work and the specific heat at constant pressure used in Wapperom and Hulsen [8] is presented for the sake of comparison.

3. The pressure equation of state

Fortunately there exists a plethora of equations of state in the literature for polymeric materials e.g. ([18–22]) and many others. The well-known Tait equation of state is used since it received wide acceptance as could be seen from the literature. The general form of the Tait equation is:

$$p(V, T) = B(T) \left[\exp\left(\frac{1 - V/V_0(T)}{a_1}\right) - 1 \right] \quad (23)$$

where V is the specific volume, a_1 is a universal constant equals to 0.0894, $B(T)$ and $V_0(T)$ are temperature-dependant constants usually take the form:

$$V_0(T) = a_2 \exp(a_3(T - 273)) \quad (24)$$

and

$$B(T) = a_4 \exp(a_5(T - 273)) \quad (25)$$

with $a_i (i = 2..5)$ are material constants e.g. for low-density polyethylene are given by Zoller [18] and Rodcers [21]:

$$a_2 = 1.1484, a_3 = 6.95E - 4, a_4 = 1929, a_5 = -4.701E - 3,$$

The isothermal speed of sound, c , for the Tait equation is:

$$c^2 = \frac{V^2(p + B(T))}{a_1 V_0(T)} \quad (26)$$

4. Heat conduction constitutive equation

When studying non-isothermal flows of polymeric fluids, one should consider not only the production of heat within the material due to viscous heating and entropic effects, but also the transport or conduction of that thermal energy from a given material point within the medium to another [16]. Assuming a Fourier-type heat conduction constitutive equation between the heat flux and the temperature gradient,

$$\mathbf{h} = -\mathbf{M} \cdot \nabla T \quad (27)$$

where \mathbf{M} is the thermal conductivity tensor. Based on non-isothermal elastic dumbbell model, Van den Brule [23] suggested the following formula for the thermal conductivity tensor for polymeric fluids:

$$\mathbf{M} = k^s \boldsymbol{\delta} + \frac{3\xi}{2m} R_p \rho \mathbf{c} \quad (28)$$

where k^s is the isotropic solvent thermal conductivity. The material parameter $\beta = m/\xi$ has the dimensions of time and unfortunately, to the best of the author's knowledge, there is no available experimental data for β . At present, only limited experimental data for the thermal conductivity of polymer melts (Venerus et al. [24]) and none for dilute solutions (van Krevelen and Nijenhuis, [25]); as well as there are no data on the effect of velocity gradients on thermal conductivity (Bird et al. [26]).

5. Numerical simulation of unsteady 1-D compression of a viscoelastic fluid

In order to numerically simulate the two experimentally-observed phenomena by Flaman and Veltman [11] during injection molding and to compare the current model with the one proposed by Wapperom & Hulsen [8]; consider a rigid tube, filled with a polymeric fluid, fastened at its left end to movable piston and at its right end to a rigid wall as shown in Fig. 1.

The fluid is divided into n zones by a Lagrangian grid. The non-dimensional Lagrangian form of the equations to be solved in its one-dimensional form is:

Conservation of mass,

$$\rho = \frac{\Delta m}{\Delta x}$$

where $\Delta m = \rho_0 \Delta x_0$ is the constant fluid mass contained in a Lagrangian zone.

Momentum equation,

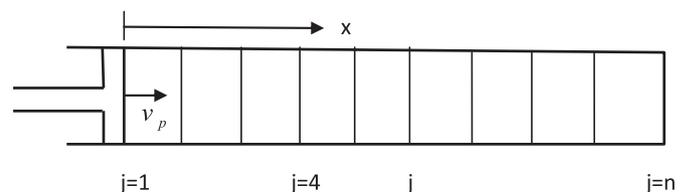


Fig. 1. Notation for the piston problem.

$$\frac{Du}{Dt} = \frac{1}{\rho} \frac{\partial \sigma_{xx}}{\partial x}$$

nodes velocity,

$$\frac{Dx}{Dt} = u$$

Equation of state, namely Equation (23),

$$p = p(V, T)$$

Compressible conformation tensor evolution equation ([12]),

$$\frac{Dc_{xx}}{Dt} + c_{xx} \left(\frac{1}{W_e(T)} - 3 \frac{\partial u}{\partial x} \right) = \frac{1}{W_e \rho f}$$

where $W_e(T) = W_{er1} \exp[-8.86(T-1)/T - 0.746]$,

with $W_{er1} = \lambda_r c_0 / L_0$,

or $W_e(T) = W_{er2} \exp[A_2 / TT_r]$,

with $W_{er2} = A_1 c_0 / L_0$

is the temperature-dependant Weissenberg number.

Temperature equation in terms of the specific volume,

$$\frac{DT}{Dt} = \frac{(\sigma_{xx} - z_\pi) DV}{z_\nu} + \frac{z_p T^2 df}{2z_\nu} \frac{Dc_{xx}}{Dt}$$

where z_p is a non-dimensional number defined as: $z_p = R_p T_r / c_0^2$

with $z_\pi = \frac{\pi}{\rho_0 c_0^2}$ and $z_\nu = \frac{c_v \epsilon T_r}{c_0^2}$

The solvent extra-stress equation is,

$$\tau_{sxx} = \left(\frac{2}{R_{es}} + \frac{1}{R_{ed}} \right) \frac{\partial u}{\partial x} = \frac{1}{R_{esd}} \frac{\partial u}{\partial x}$$

where $R_{es} = \rho_0 c_0 L_0 / \eta_s$ is the Reynolds' number based on the shear viscosity, $R_{ed} = \rho_0 c_0 L_0 / \eta_d$ is the Reynolds' number based on the dilatational viscosity and $R_{esd} = \rho_0 c_0 L_0 / (2\eta_s + \eta_d)$.

The polymer extra-stress equation is,

$$\tau_{pxx} = z_p \rho T [f c_{xx} - 1]$$

Total stress relation,

$$\sigma_{xx} = -p + \tau_{sxx} + \tau_{pxx}$$

Artificial viscosity is needed for stability reasons. The artificial viscosity introduced by Von Neumann and Richtmyer [27] uses an artificially viscous pressure, q , to spread the discontinuity front over few computational zones. The added viscous pressure is defined as:

$$q = k_1 \rho \left(\frac{\partial u}{\partial x} \Delta x \right)^2 - k_2 \rho c \frac{\partial u}{\partial x} \Delta x$$

where c is the speed of sound defined by Equation (26) and $k_1 = 0.5$, $k_2 = 4.0$ are constants.

The non-dimensionalization scheme used is:

$$\rho^* = \frac{\rho}{\rho_0}, \mathbf{v}^* = \frac{\mathbf{v}}{c_0}, p^* = \frac{p}{\rho_0 c_0^2}, T^* = \frac{T}{T_r}, t^* = \frac{t c_0}{L_0},$$

$$\boldsymbol{\sigma}^* = \frac{\boldsymbol{\sigma}}{\rho_0 c_0^2}, f^* = \frac{f(T)}{f(T_r)}, \mathbf{c}^* = \mathbf{c} f(T_r)$$

Notice that we are using $c_0(V_0, p_0)$, which is the speed of sound evaluated at initial conditions, as the reference velocity. L_0 is a reference length. The “asterisk” is dropped for clarity.

5.1. Finite difference approximation

A forward Euler scheme is used for all variables. The velocity $u(t, x)$ and the Lagrangian coordinate $x(t)$, are associated with zone boundaries j while the rest of the variables are associated with the zone centers $j + 1/2$. With the following initial and boundary conditions:

The non-dimensional initial conditions are:

$$\rho(0, x) = 1, u(0, x) = 0, T(0, x) = 1, \tau_{pxx}(0, x) = 0, c_{xx}(0, x) = 1$$

The non-dimensional boundary conditions are:

The strain-rate is defined at the left boundary as:

$d_{xx}(t, 0) = H(t)$, where $H(t)$ is the applied strain-rate. Different cases for $H(t)$ is considered. At the right boundary, $u(t, 1) = 0$ and $x(t, 1) = 1$ are imposed.

5.2. Material data

Polyethylene is selected with the following properties:

$$\pi = 3470.0 \text{ bar}, T_r = 403.15K, (\text{Dressler [12]}), B = -1.45, \lambda_r = 0.01 \text{ sec},$$

$$A_1 = 1.8984E - 7 \text{ sec}, A_2 = 4.043431E3K [6],$$

$$M_W = 0.028 \text{ kg/mol}, [25],$$

$$2\eta_s + \eta_d = 200 \text{ Pa}\cdot\text{s} \text{ (assumed)},$$

Assuming an initial pressure of 1 bar along with the reference temperature $T_r = 403.15K$ results in an initial density, using Tait equation, of $\rho_0 = 795.47 \text{ kg/m}^3$ and an initial speed of sound $c_0 = 1212.9 \text{ m/s}$.

5.3. Case a: linear loading

The applied strain-rate is $d_{xx}(t, 0) = -67.52t \text{ [s}^{-1}\text{]}$, with $L_0 = 30 \text{ cm}$, $n = 200$. With this type of loading, it is possible to study the behavior of the proposed model in regards to the temperature change as the strain-rate is increasing gradually.

Fig. 2 shows the temperature difference $[\Delta T = T(t, 0) - T(0, 0)]$ using the proposed temperature equation and using the temperature equation proposed by Wapperom and Hulslen [8] as a function of the strain-rate. As shown in the figure, Wapperom & Hulslen [8] model predicts higher temperature values as the strain-rate increases, a major cause could be deduced by noticing the predicted temperature by their model without considering the elasticity effects (purely entropic case) which produces almost exactly the same temperature distribution as for the viscoelastic case ($\gamma = 0.5$), similar behavior is noticed by Wapperom et al. [28]. This means that negligible part of the internal energy, almost zero, is stored as elastic energy. For the present model, the viscoelastic case results in a lower temperature values than for the purely entropic case. This is due to the fact that part of the internal energy is stored as elastic energy for the viscoelastic case while in the purely entropic case, all the internal energy is dissipated as heat and hence results in a higher temperature. The results of our model are more consistent with the conclusion reached by Ionescu et al. [6] about the effects of including the elasticity effects when calculating the temperature difference of a viscoelastic liquid for strain-rates approximately higher than $50 \text{ [s}^{-1}\text{]}$.

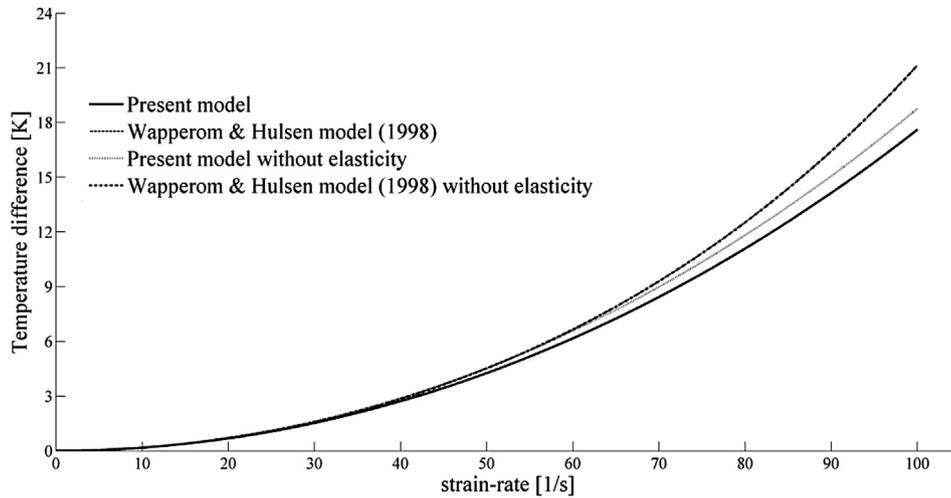


Fig. 2. Temperature distribution using the present model and Wapperom & Hulsen model (1998).

5.4. Case b: impulsive loading

In injection molding, where the pressure is increased by a few hundred bars in a short time, the temperature rise due to compression effects plays an important role as noticed by Flaman and Veltman [11]. This effect is well-known for gases, but also for polymeric fluids it is often not negligible as noticed by Wapperom [29]. In this subsection, the temperature rise due to sudden compression is studied as well as the time-lag of the induced pressure waves.

The applied strain-rate is: $d_{xx}(t, 0) = d_{xx}^{max}\delta(t)$, with $L_0 = 30$ cm, $n = 400$. Where $\delta(t)$ is the Dirac-delta function, with this type of loading we can study the two main observations made by Flaman and Veltman [11] during injection molding, namely, the temperature rise due to compression effects resulting from a change in pressure by few hundred Bars, in a short time as well as the time delay between the action of loading and the first arrival of the signal at any spatial position e.g. pressure transducer location. The following results are for $d_{xx}^{max} = -1E5 s^{-1}$ or (-24.73 non - dimensional) with the numerical representation of the Dirac-delta function is:

$$\delta(t) = \begin{cases} 1 & 0 \leq t \leq \Delta t \\ 0 & t > \Delta t \end{cases}$$

Fig. 3 shows the pressure difference ($p(t, x) - p(0, x)$), distribution along the piston axis for different times in [Bars]. The time-lag observed by Flaman and Veltman [11] during a similar compression

is so clear here e.g. a pressure transducer located say at $x \approx 0.8$ would not feel any difference until the wave reaches its location after $t \approx 0.55$.

The corresponding temperature increase is shown in Fig. 4, which shows approximately $\Delta T \approx 15$ [K] as result of $\Delta p \approx 325$ [Bars] which is consistent with the second observation made by Flaman and Veltman [11]. It is worth noting how is the pressure as well as the temperature abrupt changes are very well captured without any oscillations due to the use of the artificial viscosity introduced by Von Neumann and Richtmyer [27].

6. Summary and conclusion

With a simple modification to the Massieu thermodynamic potential, a temperature equation for polymeric fluids is derived with the explicit appearance of the elasticity as well as compressibility effects. One of the advantages of the proposed temperature equation is that it does not contain functions that depend on the stress-models. To close the system of equations, the Tait equation of state is used to relate the thermodynamic pressure to the specific volume and the temperature. An unsteady Lagrangian finite difference scheme is used to investigate numerically, the experimentally-observed phenomena by Flaman and Veltman [11] namely, the temperature rise due to sudden increase in the pressure by few hundred Bars and the time delay in measuring the pressure during the injection molding. As a second test case, the proposed temperature equation is tested against the one proposed by Wapperom and Hulsen [8] and the results of the simulation

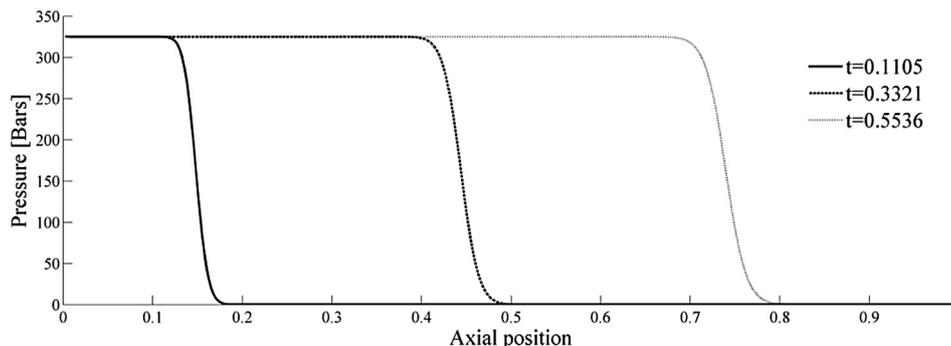


Fig. 3. Pressure difference distribution along the piston axis at different times.

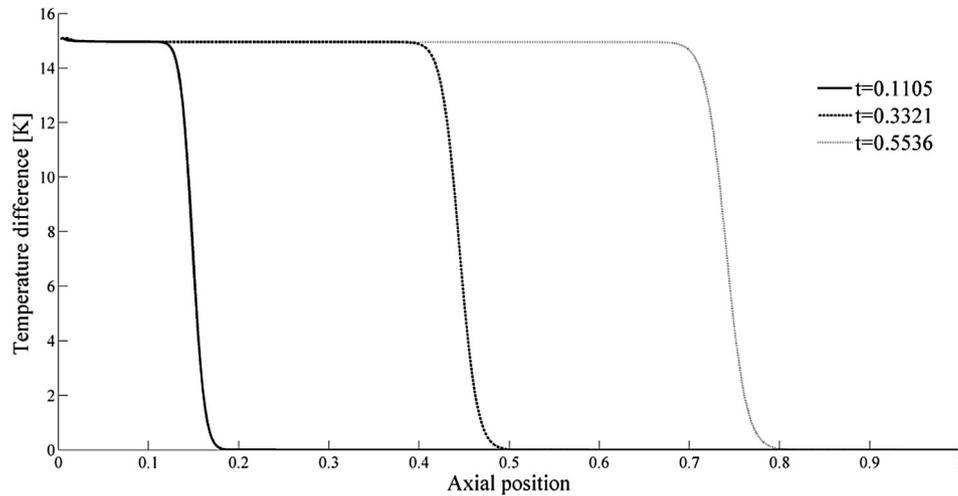


Fig. 4. Temperature difference distribution along the piston axis at different times.

show that the proposed model accounts better for the elasticity of the fluid.

Appendix A. Temperature equation of Wapperom and Hulslen (1998)

A temperature equation for compressible viscoelastic fluids has been derived from thermodynamics in Wapperom [29] and Wapperom and Hulslen [8]. For Oldroyd fluid (Wapperom et al. [28]):

$$\rho c_{p,\mathbf{b}} \frac{DT}{Dt} = \beta T \frac{Dp}{Dt} - \nabla \cdot \mathbf{h} + Q \quad (\text{A1})$$

where:

$$Q = \gamma \tau : \mathbf{d} + (1 - \gamma) D_m \quad (\text{A2})$$

and

$$D_m = \tau_s : \mathbf{d} + \frac{\rho T^\gamma}{2\lambda(T)} (\text{tr} \mathbf{b} + \text{tr} \mathbf{b}^{-1} - 2\delta_{ii}) \quad (\text{A3})$$

where \mathbf{b} is the configuration tensor, $c_{p,\mathbf{b}}$ is the specific heat at constant pressure and configuration tensor \mathbf{b} , and γ is the energy partitioning coefficient such that:

$$\begin{aligned} \gamma = 0 & : \text{pure energy elasticity} \\ \gamma = 1 & : \text{pure entropy elasticity} \end{aligned}$$

The evolution equation for the configuration tensor is:

$$\lambda(T) \left(\frac{d\mathbf{b}}{dt} - \mathbf{Ib} - \mathbf{bI}^T \right) + \mathbf{b} = \delta \quad (\text{A4})$$

and the polymer stress is defined as:

$$\tau_p = \rho T^\gamma (\mathbf{b} - \delta) \quad (\text{A5})$$

From the fundamentals of thermodynamics:

$$c_{p,\mathbf{b}} - c_{V,\mathbf{c}} = T \left. \frac{\partial p}{\partial T} \right|_V \left. \frac{\partial V}{\partial T} \right|_p \quad (\text{A6})$$

The Tait equation is used to find the partial derivatives of the right hand side of the above equation (A6) as:

$$\left. \frac{\partial p}{\partial T} \right|_V = a_5 p + \frac{a_3 V}{a_1 V_0(T)} (p + B) \quad (\text{A7})$$

$$\left. \frac{\partial V}{\partial T} \right|_p = a_3 V + a_1 a_5 V_0(T) \frac{p}{p + B} \quad (\text{A8})$$

for low-density polyethylene; $\beta = 7.02E - 4$ [1/K] taken from Wapperom and Hulslen [8]. For comparison purposes with the present model, Equation (A6), along with (A7) and (A8), is used for the numerical simulation.

References

- [1] W.C. Ko, D.C. Bogue, A constitutive equation including compressibility effects, *J. Rheol.* 31 (1987) 425–438.
- [2] G. Astarita, Thermodynamics of dissipative materials with entropic elasticity, *Polym. Eng. Sci.* 14 (1974) 730–733.
- [3] G. Astarita, G.C. Sarti, The dissipative mechanism in flowing polymers: theory and experiments, *J. Non Newton. Fluid Mech.* 1 (1976a) 39–50.
- [4] G. Astarita, Sarti, GC, approach to thermodynamics of polymer flow based on internal state variables, *Polym. Eng. Sci.* 16 (1976b) 490–495.
- [5] G.C. Sarti, N. Esposito, Testing thermodynamic constitutive equations for polymers by adiabatic deformation experiments, *J. Non Newton. Fluid Mech.* 3 (1977) 65–76.
- [6] T.C. Ionescu, B.J. Edwards, D.J. Keffer, V.G. Mavrantzas, Energetic and entropic elasticity of nonisothermal flowing polymers: experiment, theory, and simulation, *J. Rheol.* 52 (1) (2008) 105–140.
- [7] A. Wachs, Clermont, JR, isothermal viscoelastic flow computations in an axisymmetric contraction at high Weissenberg numbers by a finite volume method, *J. Non Newton. Fluid Mech.* 95 (2000) 147–184.
- [8] P. Wapperom, M.A. Hulslen, Thermodynamics of viscoelastic fluids: the temperature equation, *J. Rheol.* 42 (1998) 999–1019.
- [9] M. Grmela, D. Jou, J. Casas-Vazquez, Nonlinear and Hamiltonian extended irreversible thermodynamics, *J. Chem. Phys.* 108 (1998) 7945–7973.
- [10] M. Grmela, Letter to the editor: comment on “thermodynamics of viscoelastic fluids: the temperature equation” [*J. Rheol.* 42, 999–1019 (1998)], *J. Rheol.* 42 (1998) 1565–1567.
- [11] A.A.M. Flaman, B. Veltman, Injection moulding experiments, a challenge to numerical simulation programs, *Rheol. Acta* 26 (1988) 129–131.
- [12] M. Dressler, The Dynamical Theory of Non-Isothermal Polymeric Materials, Ph.D. Dissertation, ETH, Zurich, 2000.
- [13] M. Grmela, Hamiltonian mechanics of complex fluids, *J. Phys. A* 22 (1989) 4375–4394.
- [14] A.N. Beris, B.J. Edwards, Thermodynamics of Flowing Systems, in: A.L. Cullen, L.C. Woods, et al. (Eds.), Oxford University Press, Oxford, UK, 1994, pp. 114–118.
- [15] H.C. Öttinger, M. Grmela, Dynamics and thermodynamics of complex fluids: II. Illustrations of a general formalism, *Phys. Rev. E* 56 (1997) 6633–6655.
- [16] M. Dressler, B.J. Edwards, H.C. Öttinger, Macroscopic thermodynamics of flowing polymeric liquids, *Rheol. Acta* 38 (1999) 117–136.
- [17] R.K. Gupta, A.B. Metzner, Modeling of non-isothermal polymer processes, *J. Rheol.* 26 (1982) 181–198.

- [18] P. Zoller, The pressure-volume-temperature properties of three well-characterized low-density polyethylenes, *J. Appl. Polym. Sci.* 23 (1979) 1051–1056.
- [19] B. Cho, Equations of state of polymer, *Polym. Eng. Sci.* 25 (18) (1985) 1139–1144.
- [20] G.T. Dee, T. Ougizawa, D.J. Walsh, The pressure-volume-temperature properties of polyethylene, poly(dimethyl siloxane), poly(ethylene glycol) and poly(propylene glycol) as a function of molecular weight, *Polymer* 33 (16) (1992) 3462–3469.
- [21] P.A. Rodgers, Pressure-volume-temperature relationships for polymeric liquids: a review of equations of state and their characteristic parameters for 56 polymers, *J. Appl. Polym. Sci.* 48 (1993) 1061–1080.
- [22] I.C. Sanchez, J. Cho, A universal equation of state for polymer liquids, *Polymer* 36 (15) (1995) 2929–2939.
- [23] B.H.A.A. Van den Brule, The non-isothermal elastic dumbbell: a model for the thermal conductivity of a polymer solution, *Rheol. Acta.* 29 (1990) 416–422.
- [24] D.C. Venerus, J.D. Schieber, V. Balasubramanian, K. Bush, S. Smoukov, Anisotropic thermal conduction in a polymer liquid subjected to shear flow, *Phys. Rev. Lett.* 93 (9) (2004) 1–4.
- [25] D.W. Van Krevelen, K. Te Nijenhuis, *Properties of Polymers*, fourth ed., Elsevier, Amsterdam, 2009.
- [26] R.B. Bird, C.F. Curtiss, K.J. Beers, Polymer contribution to the thermal conductivity and viscosity in a dilute solution (Fraenkel Dumbbell model), *Rheol. Acta.* 36 (1997) 269–276.
- [27] J. Von Neumann, R.D. Richtmyer, A method for the numerical calculation for hydrodynamic shocks, *J. Appl. Phys.* 21 (1950) 232–237.
- [28] P. Wapperom, M.A. Hulsen, J.P.P.M. Van der Zanden, A numerical study for steady and non-isothermal viscoelastic fluid for high Deborah and Peclet numbers, *Rheol. Acta* 37 (1998) 119.
- [29] P. Wapperom, *Nonisothermal Flows of Viscoelastic Fluids: Thermodynamics, Analysis and Numerical Simulation*, PhD dissertation, Delft University of Technology, 1995.