Finite Elements Approximate Flows of Compressible Viscous Melt Molecules

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Abstract

This paper is aimed to obtain results on flow of a class of compressible viscous polymer melt molecules when state frequency transition is assigned and finite elements considered as basis of flow analysis. When frequency error was related to to local error, arising from finite elements scheme, it was revealed that extent of energy corrections was directly proportional to the flow tolerance level. The processing over flow encountered while generating finite elements was assumed to arise as a result of increasing wave interference. Although the flow frequency was found to be increasing, it was insufficient for improving the prescribed energy level. Conclusively, it was assumed that the flow of the fluid being examined was naturally irregular.

Keywords: Transition states assignment, Response sensitivity determinants, Finite elements approximate, Energy correction.

1.0 Introduction

Let E be a measure of heat energy and e(t) be internal heat correction. Then the corrected form of the theoretical heat energy equation arising from flow of a class of compressible viscous polymer melt molecules is prescribed by

$$d[\rho(E(r, \theta, t) – e(t))]/dt = \rho(E(r, \theta, t) – e(t)) - \rho \blacktriangledown (E(r, \theta, t) – e(t)) + y \blacktriangledown^2 v(r, \theta, t),$$
$$\rho = \rho(t) \tag{1.1}$$

where ρ is the melt density, y is the melt viscosity, v is the flow velocity and $\blacktriangledown = (r\partial/\partial r, \partial/\partial \theta)$ is a differential operator [1]. Suppose equation (1.1) is subject to initial and boundary conditions [2]

$$E(r, \theta, t) = E_1(r, \theta), \partial E(r, \theta, t)/\partial t = 0; 1 < r < \alpha, 0 < \theta < 1, t > 0 \tag{1.2}$$

$$E(1, 0, t) = E_2(t) > E_1(r, \theta), E(\alpha, 1, t) = 0, t > 1 \tag{1.3}$$

Meanwhile, let the flow frequency error of the molecules be

$$J = \int_0^1 \Phi(E, e, t)dt \tag{1.4}$$

Also let Δp, ΔV and ΔT be corrections to pressure, volume and temperature correspondingly. Then the corrected version of gas law version [3] is given by

$$(p - \Delta p)(V - \Delta V) = R_0(T + \Delta T), T = T(r, \theta, t) – T_0 \tag{1.5}$$

For applications, choose

$$E(r, \theta, t) = \rho T/(R_0 \alpha^2), E = \rho(E(r, \theta, t) – e(t)) \tag{1.6}$$

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Equations (1.1) - (1.3) yield energy states transition equations

$$dE/dt - L(E, E) = \mathrm{y}\blacktriangledown^2 v(r, \theta, t), \quad L = (\rho, -\rho\blacktriangledown)$$
$$= 0, \quad \rho(0) = \rho_0 \tag{1.7}$$

such that

$$E/\rho + e(t) = \rho T/(R_0\alpha^2), \quad \lim_{t\to\infty} e(t) = 0 \tag{1.8}$$

$$E = E_1, \quad t = 0; \quad \partial E/\partial t = 0, \quad 1 < r < \alpha, \quad 0 < \theta < 1, \quad t > 0 \tag{1.9}$$

$$E = E_2 > E_1, \quad r = 1, \quad \theta = 0, \quad t >= 0; \quad E = 0, \quad r = \alpha, \quad \theta = 1, \quad t > 1 \tag{1.10}$$

2.0   Energy Correction

Let A be L-associated Hessian of J [4]. If A is singular [5], then choose sensitivity response λ to be its robust characteristic value and μ to be the corresponding tolerance index [6], [7]. If (r*, θ*) is the corresponding characteristic vector of A, then regular flow frequency Fr is ensured such that

$$Fr = [r^*, \theta^*][d/dt - (A - \lambda I)][r^*, \theta^*]^T \tag{2.1}$$

Borrowing idea from Maroni 1994 [8], the product

$$< \mu, \lambda > = 1/m \int_o^t p(v)p^*(v)dt$$
$$= \delta_{ij}, \quad m = 1/t \int_o^t vp(v)dt \tag{2.2}$$

Such that p* is the orthogonal conjugate of the polynomial p. The foregoing constitutes flow stability analysis which is naturally endowed with corrected

$$\mathrm{y}\blacktriangledown^2 v(r, \theta, t) = \mu\delta_{ij}Fr \tag{2.3}$$

$$E^* = E + Fr \tag{2.4}$$

$$J = \int_0^1 \Phi(E^*, e, t)dt \tag{2.5}$$

3.0   Approximate Finite Elements

Consider equations (1.8)-(1.10) and for solution, choosing step length $\Delta r = \Delta\theta = h$ for the difference scheme

$$\partial E^{k+1} = cq[E_{i+1, j}{}^k - 2E_{i, j}{}^k + E_{i, j+1}{}^k] \quad E^k = \partial^k E/\partial t^k \tag{3.1}$$

such that $q = \Delta t/h$, $c = q(1 + q/2)$ and local error

$$LE = c(h + 2h^2) \tag{3.2}$$

With selections of $\Delta t = 0.2$ and $h = 0.5$, one obtains $q = 0.4$, $c = 0.48$ and $LE = 0.192$ The process adopted in generating the values in table 3.1 is illustrated in figure 3.1.
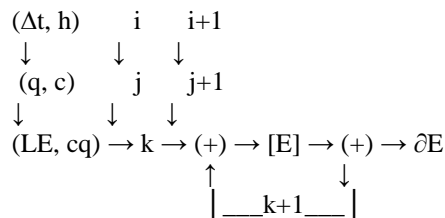
```
(Δt, h)     i     i+1
 ↓          ↓     ↓
(q, c)      j     j+1
 ↓          ↓     ↓
(LE, cq) → k → (+) → [E] → (+) → ∂E
                ↑           ↓
                | __k+1__ |
```

Figure 3.1: Illustration of procedure for generation of finite elements. The process of calculation is progressively top

downwards followed by left rightwards according to arrow directions indicated. Task is updated in lower feedback loop such that k=k+1 requests for readiness for next cycle of the task.

Table 3.1: Calculated sample values

k	t	i, j	e(t)	$E_{i,j}^{k}$	$E_{i+1,j}^{k}$	$E_{i,j+1}^{k}$
0	0.0	0	1.92E-01	0.0	0.5	1.0
1	0.2	1	1.92E-02	0.2	0.2	0.2
1	0.4	2	1.92E-02	0.2	0.2	0.2
2	0.4	2	1.92E-03	0.4	0.4	0.4
3	0.6	2	1.92E-04	0.6	-	-
4	0.8	1	1.92E-05	0.8	-	-
5	1.0	0	1.92E-06	1.0	-	-
.	...	.	....	...	.	.

For discussions, chose $\lambda = \lambda_{max}$, $\mu = \lambda_{max}10^{-k}$ and
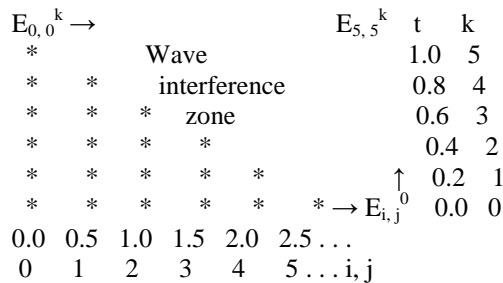
$$J = (10(E - Fr^2))^2 + (1 - Fr)^2 \tag{3.3}$$

When J was subjected to minimization procedure [9], the values in table 3.2 were obtained.

Table 3.2: Calculated sample values

k	E	Fr	J	μ
0	0.17223	0.30984	1.057350	1E-00
1	0.14223	0.30384	1.037250	1E-01
2	0.43684	0.60401	0.675310	1E-01
3	0.47799	0.68632	0.103242	1E-02
4	0.48375	0.69783	0.092343	1E-03
5	0.48383	0.69800	0.092341	1E-04
.	....	....	....	.....

4.0   Discussion of Results

The value of internal energy correction e(t) was calculated as the product of tolerance value and local error value (e(t)= < μ, LE >). The calculated values were found to be progressively vanishing as the tolerance index (see table 3.1) 2D-plot of the values of E is given in figure 4.1.

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E_0,0^k →                        E_5,5^k   t    k
   *                  Wave            1.0   5
   *      *        interference       0.8   4
   *      *    *      zone            0.6   3
   *      *    *     *                    0.4   2
   *      *    *     *    *           ↑   0.2   1
   *      *    *     *    *     * → E_i,j^0   0.0   0
0.0  0.5  1.0  1.5  2.0  2.5 ...
 0    1    2    3    4    5 ... i, j
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Figure 4.1: A 2-D plot of values of E. Non zero values denoted by asterisks (*) are situated in the lower triangular region while the zero values are situated in the upper triangular region. From technical point of view, such zero values are taken to be due to the prevailing wave interference.

5.0   Conclusion

Judging from the pattern exhibited by table values, the prevailing energy correction e(t) is directly proportional to the flow tolerance index μ. When i=j at k > 2, processing of values of E over flew (see table 3.1). This situation was assumed to be so due to increasing wave interference (see figure 4.1). Although the flow frequency Fr was increasing, it was insufficient for improving the prescribed energy level E in equation (3.1). Thus it is likely that the investigated flow of the compressible viscous polymer melt is naturally irregular.

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