The free (open) boundary condition with integral constitutive equations

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Abstract

The free (open) boundary condition (FBC, OBC) was proposed by Papanastasiou et al. (A new outflow boundary condition, Int. J. Numer. Methods Fluids 14 (1992) 587–608) to handle truncated domains with synthetic boundaries where the outflow conditions are unknown. In the present work, implementation of the FBC has been extended to viscoelastic fluids governed by integral constitutive equations. As such we consider here the K-BKZ/PSM model, which also reduces to the upper-convected Maxwell fluid (UCM) for a single relaxation time and an appropriate choice of material parameters. The Finite Element Method (FEM) is used to provide numerical results in simple test cases, such as planar flow at an angle and Poiseuille flow in a tube where analytical solutions exist for checking purposes. Then previous numerical results obtained with the differential UCM model are checked in highly viscoelastic flows in a 4:1 contraction. Finally, the FBC is used with the K-BKZ/PSM model with data corresponding to a benchmark polymer melt (the IUPAC-LDPE melt). Particular emphasis is based on a non-zero second normal-stress difference, which has been reported in the literature to cause problems and seems responsible for earlier loss of convergence. The results with the FBC in short domains are in excellent agreement with those obtained from long domains used until now to accommodate the highly convective nature of the stresses in viscoelastic flows, for which the FBC seems most appropriate.

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1. Introduction

The free (open) boundary condition (FBC, OBC) was proposed by Papanastasiou et al. [1] to handle truncated domains with synthetic boundaries where the outflow conditions are unknown. This came in response to a concerted effort some 20 years ago to solving the problem of boundary conditions at outflows, in a symposium entitled “Minisymposium on Outflow Boundary Conditions for Incompressible Flow”, which took place on July 14, 1991 at the University of California at Davis [2]. In the minisymposium, the OBC proposed by Papanastasiou et al. [1] was given plaudits for impressively accurate results for the benchmark Backward-Facing Step (BFS) problem [3] and Stratified Backward-Facing Step (SBFS) problem [4], and the method was also implemented by others for the same problem with equally good results.

The original idea by Papanastasiou et al. [1] has been implemented also for free-surface flows by Malamataris [5], and Malamataris and Papanastasiou [6]. Since then, several papers have appeared in the literature on the subject [7–11], sometimes referring to the FBC as an “open boundary condition” [4] or a “synthetic outflow boundary condition” [1] or a “no boundary condition” [7,8]. The mathematics behind its workings has also been explained [1,7,8]. It seems that the method has been implemented in several computational codes for fluid mechanics, and in many papers there is a passing mentioning of its application as part of the solution, e.g., [12]. However, details about its implementation in other linear-system solution schemes (like Picard iterations) and a more careful formulation was given in some detail for fixed-point iterative schemes (like Picard iterations) and a more careful analysis of the results, especially regarding individual effects of various fluid mechanics parameters, as well as the outflow pressures – a sensitive quantity – appears missing from the literature.

The authors have improved on this in a recent paper [13] by revisiting the original benchmark viscous problems (BFS and SBFS) and showing detailed results for the primary variables (velocities–pressures–temperatures). Furthermore, they have also applied it to the benchmark free-surface problem of extrudate-swell for Newtonian fluids [14,15]. The Finite Element Method (FEM) was used to provide and compare numerical results with previous solutions [1–4]. The formulation was given in some detail for fixed-point iterative schemes (Picard iteration) as opposed to Newton–Raphson schemes, with regard to computational aspects. Some interesting conclusions from the recent work [13] showed that when the outflow BC is known (as with surface tension effects in extrudate swell), then the FBC is not needed and should not be used; also for vertical extrusion under gravity, the FBC is not valid, since the body force due to gravity always adds a force and the domain cannot be truncated.

For viscoelastic flows, which admittedly are more difficult to solve due to the highly non-linear nature of the rheological
constitutive equation for the stresses, the implementation of FBC has also been used. Park and Lee [10] appear to be the first to have used it with the differential upper-convected Maxwell model (UCM) in isothermal and non-isothermal flows. Then Sunwoo et al. [11] extended the method to three-dimensional coextrusion flows with the differential Phan-Thien/Tanner model with good results. Dimakopoulos and Tsamopoulos [12] have also used it with the differential Giesekus model, which may exhibit a second normal-stress difference \( N_2 \). These authors found that when \( N_2 \neq 0 \), it was necessary to impose \( \partial u / \partial z = 0 \) on the FBC in order to get correct results, i.e., a parallel flow at the die outlet [12].

In view of the above findings, the present authors decided to further study the FBC for viscoelastic fluids. In a recent paper [16] they have used the FBC with differential viscoelastic models of the Criminal–Ericksen–Filbey (CEF) type [14], which give the stress tensor explicitly as a function of the strain-rate tensor. These models reduce to the second-order fluid (SOF), which has analytical solutions in simple flows [14]. It was then possible to successfully check the results against analytical solutions in the presence of the extra stress tensor, \( \sigma \). Dimakopoulos and Tsamopoulos [12] have also used it with flows with the differential Phan-Thien/Tanner model with good results. Then Sunwoo used it with the differential upper-convected Maxwell model with good results given by Park and Lee [10].

In the present work, we continue along the same lines by studying integral constitutive equations of the K-BKZ type [14], where the FBC has not been addressed so far in its full implementation. These rheological models have been found to represent accurately polymer solutions and melts by employing a spectrum of relaxation times [26,27] and will not be repeated here. Suffice to say that the FBC works well for these models as well, so that shorter domains can be used in the simulations. First we establish the validity of our formulation in simple test flows with the integral equivalent of the upper-convected Maxwell fluid with or without a second normal-stress difference \( N_2 \). Then we embark on solving the integral K-BKZ viscoelastic model in flow through an abrupt contraction, for which in the past very long domains were used to fully relax the high viscoelastic stresses in the die [20–23]. Particular emphasis is based on obtaining valid results with a non-zero \( N_2 \), which in the past plagued the implementation of FBC leading to ad hoc remedies [12]. The efficiency of the FBC for truncated domains will be shown in comparison with results from longer dies.

2. Mathematical modeling

2.1. Governing equations

We consider the conservation equations of mass, momentum and energy for incompressible fluids under non-isothermal, creeping, steady flow conditions. These are written as [14]:

\[ \nabla \cdot \vec{u} = 0, \]  
\[ \rho \vec{u} \cdot \nabla \vec{u} = -\nabla p + \nabla \tau, \]  
\[ \rho C_p \vec{u} \cdot \nabla T = k \nabla^2 T + \tau : \nabla \vec{u}, \]  

where \( \rho \) is the density, \( \vec{u} \) is the velocity vector, \( p \) is the pressure, \( \tau \) is the extra stress tensor, \( T \) is the temperature, \( C_p \) is the heat capacity, and \( k \) is the thermal conductivity.

Viscoelasticity is included in the present work via an integral rheological model for the stresses. This is a K-BKZ model proposed by Papastasiou et al. [24] and modified by Luo and Tanner [25]. It is written as:

\[ \tilde{\tau} = \frac{1}{1 - \theta} \int_{-\infty}^{t - \theta} \sum_{k=1}^{N} \frac{\alpha_k}{\beta_k} \exp \left( -\frac{t - \tau}{\lambda_k} \right) \frac{\alpha}{(\lambda - 3) + \beta_k \lambda_k} \tilde{\tau}^{-1}(\tau) \]  
\[ + \theta \tilde{\tau}(t) \, dt', \]  

where \( \lambda_k \) and \( \alpha_k \) are the relaxation times and relaxation modulus coefficients, respectively, \( N \) is the number of relaxation modes, \( \alpha \) and \( \beta \) are material constants, and \( \lambda_k \) are the first invariants of the Cauchy–Green tensor \( \tilde{C} \) and its inverse \( \tilde{C}^{-1} \), the Finger strain tensor. The material constant \( \theta \) is given by

\[ \frac{N_1}{N_2} = \frac{\theta}{1 - \theta}, \]  

where \( N_1 \) and \( N_2 \) are the first and second normal stress differences, respectively. It is noted that \( \theta \) is not zero for polymer melts, which possess a non-zero second normal stress difference. Its usual range is between \(-0.1\) and \(-0.2\) in accordance with experimental findings [14].

The non-isothermal version of the K-BKZ model is given in detail in [26,27] and will not be repeated here. Suffice to say that the variations of viscosity and relaxation time with temperature are modeled by using a temperature shifting function, \( \alpha_k \):

\[ \eta(T) = \eta(T_0) \alpha_k(T), \]  
\[ \lambda(T) = \lambda(T_0) \alpha_k(T), \]  

where \( \eta(T_0) \) and \( \lambda(T_0) \) are the values of viscosity and relaxation time at the reference temperature \( T_0 \), respectively. For the temperature shifting function \( \alpha_k \), an Arrhenius-type equation is used:

\[ \alpha_k(T) = \exp \left[ \frac{E_k}{k_0} \left( \frac{1}{T} - \frac{1}{T_0} \right) \right], \]  

where \( E_k \) is the activation energy of the material, representing the temperature dependence of the rheological properties, and \( k_B \) is the ideal gas constant. The temperatures are the absolute temperatures given in \( K \).

The integral model (Eq. (4)) has been used both in its isothermal and non-isothermal version for simulating the flow of a benchmark polymer melt, a low-density polyethylene (LDPE) melt, which was thoroughly characterized rheologically by an IUPAC working group [28], hence its name IUPAC-LDPE (sample A) melt. The rheological constants of the K-BKZ model and other relevant material parameters that fit data for this melt are given in Tables 1 and 2. It is seen that a relaxation spectrum is used with 8 relaxation times. The relaxation spectrum is used to find the average relaxation time, \( \bar{\lambda} \), and zero-shear-rate viscosity, \( \eta_0 \), according to the formulas:

\[ \bar{\lambda} = \frac{\sum_{k=1}^{N} \alpha_k \lambda_k^{2}}{\sum_{k=1}^{N} \alpha_k \lambda_k}, \]  
\[ \eta_0 = \sum_{k=1}^{N} \alpha_k \lambda_k. \]

The values of these parameters are \( \bar{\lambda} = 58.7 \text{ s}, \eta_0 = 51,064 \text{ Pa s} \), indicating a highly elastic melt with a long average relaxation time.

It should be noted that the K-BKZ model reduces to the Newtonian and upper-convected Maxwell (UCM) model with an appro-

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**Table 1**

<table>
<thead>
<tr>
<th>( k )</th>
<th>( \lambda_k ) (s)</th>
<th>( \alpha_k ) (Pa s)</th>
<th>( \beta_k ) (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>( 10^{-4} )</td>
<td>1.29 \times 10^{5}</td>
<td>0.018</td>
</tr>
<tr>
<td>2</td>
<td>( 10^{-3} )</td>
<td>9.48 \times 10^{4}</td>
<td>0.018</td>
</tr>
<tr>
<td>3</td>
<td>( 10^{-2} )</td>
<td>5.86 \times 10^{4}</td>
<td>0.08</td>
</tr>
<tr>
<td>4</td>
<td>( 10^{-1} )</td>
<td>2.67 \times 10^{4}</td>
<td>0.12</td>
</tr>
<tr>
<td>5</td>
<td>( 10^{0} )</td>
<td>9.80 \times 10^{3}</td>
<td>0.12</td>
</tr>
<tr>
<td>6</td>
<td>( 10^{1} )</td>
<td>1.89 \times 10^{3}</td>
<td>0.16</td>
</tr>
<tr>
<td>7</td>
<td>( 10^{2} )</td>
<td>1.80 \times 10^{2}</td>
<td>0.03</td>
</tr>
<tr>
<td>8</td>
<td>( 10^{3} )</td>
<td>1.00 \times 10^{2}</td>
<td>0.002</td>
</tr>
</tbody>
</table>
Table 2
Material parameters used in the non-isothermal simulations for the flow of the IUPAC-LDPE (sample A) melt at 150 °C [26,27].

<table>
<thead>
<tr>
<th>Parameter (symbol)</th>
<th>Value (units)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density ($\rho$)</td>
<td>918 kg/m$^3$</td>
</tr>
<tr>
<td>Specific heat ($c_p$)</td>
<td>2.302 kJ/kg K</td>
</tr>
<tr>
<td>Thermal conductivity ($k$)</td>
<td>0.26 W/m K</td>
</tr>
<tr>
<td>Activation energy ($E$)</td>
<td>57,500 J/mol</td>
</tr>
<tr>
<td>Ideal gas constant ($R_g$)</td>
<td>8.3143 J/mol K</td>
</tr>
<tr>
<td>Reference temperature ($T_a$)</td>
<td>423 K (150 °C)</td>
</tr>
<tr>
<td>Viscosity ($\eta$)</td>
<td>55,000 Pa s</td>
</tr>
<tr>
<td>Relaxation time ($\tau$)</td>
<td>0.1 s</td>
</tr>
<tr>
<td>Die radius ($R$)</td>
<td>1 cm</td>
</tr>
</tbody>
</table>

Peclet number and the Nahme–Griffith number, $Na$. These are defined as:

\[
Pe = \frac{\rho c_p U R}{k},
\]

\[
Na = \frac{\eta EU^2}{k R T_0},
\]

where $\eta = f(U/R)$ is a nominal viscosity given by the constitutive model (Eq. (4)) at a nominal shear rate of $U/R$. The Pe number represents the ratio of heat convection to conduction, and the Na number represents the ratio of viscous dissipation to conduction and indicates the extent of coupling between the momentum and energy equations. When $Pe \gg 1$, there is strong convection, while when $Na \approx 1$, there is a moderate coupling between momentum and energy equations. A value of $Na > 1$ indicates temperature non-uniformities generated by viscous dissipation, and a strong coupling between momentum and energy equations.

The above rheological model (Eq. (4)) is introduced into the conservation of momentum (Eq. (2)) and closes the system of equations. Boundary conditions are necessary for the solution of the above system of equations. These depend on the problem at hand and will be given in the appropriate place. Suffice to say that the outflow boundary condition is either a fully developed flow or the free (open) boundary condition (FBC).

All lengths are scaled by $R$, all velocities by $U$, all pressures and stresses by $\eta_0 U/R$, where $\eta_0$ is the zero-shear-rate viscosity.

3. Method of solution

The numerical solution is obtained with the Galerkin/Finite Element Method (GFEM), using a program which employs as primary variables the two velocities, pressure, and temperature ($u$–$v$–$p$–$T$ formulation) [30]. GFEM casts the differential equations into integral form according to the Galerkin principles [31,32]. For the $u$–$v$–$p$–$T$ formulation, GFEM approximates the field variables for the velocities $u$–$v$, pressure $p$, and temperature $T$, as follows:

\[
u = \phi^U \sum_{i=1}^{n} \phi_i U_i, \quad v = \phi^V \sum_{i=1}^{n} \phi_i V_i, \quad p = \phi^T \sum_{i=1}^{m} \phi_i T_i,
\]

The relevant choice of parameters. Thus, for the Newtonian fluid we either set the elastic stresses to zero and keep only the viscous (reference) stresses or we set $N = 1, \alpha_1 = 0$. For the UCM, we set $N = 1, \alpha_1 = 1, \alpha = 10,000$ and $\beta_1 = 0.001$ [29], while the viscoelastic level is set by setting $\lambda$, and this gives rise to the Weissenberg number, $Ws$, defined by:

\[
Ws = \lambda \frac{4U}{R},
\]

where $\lambda$ is the apparent shear rate (=$U/R$), $U$ is the average velocity in fully-developed flow in the die, and $R$ is the die radius. For the Newtonian fluids, $Ws = 0$.

However, for polymer melts with a spectrum of relaxation times as is the case with the LDPE melt, the Weissenberg number is not a good indication of the level of viscoelasticity. A better criterion of the viscoelastic nature of a polymeric liquid is given by the stress ratio ($S_R$), which can be shown to be equivalent to the Weissenberg number upon an appropriate choice of the material constants [19,22]. For this we write:

\[
S_R = \frac{N_1}{2\tau_w} = \frac{\Psi_1 \tau_w^2}{2\eta \tau_w} = \frac{\Psi_1}{2\eta} \lambda \tau_w,
\]

where $N_1$ is the first normal stress difference and $\tau_w$ is the shear stress both evaluated at the die wall, $\Psi_1$ is the first normal stress coefficient, and $\lambda$ is the shear rate at the die wall. Both $\Psi_1$ and $\eta$ are functions of $\lambda$ for polymer melts.

The various thermal and flow parameters are combined to give appropriate dimensionless numbers [26,27]. The relevant ones here are the Peclet number, $Pe$, and the Nahme–Griffith number, $Na$. These are defined as:

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\]
where $\mathbf{U}, \mathbf{V}, \mathbf{P}, \mathbf{T}$ are arrays-columns of the nodal unknowns for each element, and $\psi, \phi$ are arrays-rows of the basis (interpolation) functions, and the superscript $T$ refers to the transpose of a vector. The pressure basis functions $\psi$ are of a lower order than the other basis functions $\phi$, and interpolation for pressure is carried out over $m$ nodes, while for the other variables is carried over $n$ nodes, with $m < n$. The code uses Lagrangian isoparametric quadrilateral elements of the serendipity kind (8 nodes/element) [30]. This choice fixes the basis functions to $n = 8, m = 4$. Hence, the basis functions $\phi$ and $\psi$ are quadratic and linear, respectively.

Fig. 2. Pressure-driven flow of a Newtonian fluid in a planar channel at a 45°-angle with the horizontal: (a) finite element grid, (b) velocity vectors, (c) $u_x$-contours $U$, (d) $u_y$-contours $V$, (e) streamlines $\text{STR}$, (f) isobars $P$. Results by applying the FBC at outflow show that the flow develops properly to the exit.
The governing equations, weighted integrally with the basis functions, result in the following continuity, $R_{C}$, momentum, $R_{M}$, and energy, $R_{E}$, residuals in the domain $\Omega$ [1]:

$$R_{C} = \int_{\Omega} \nabla \cdot \mathbf{u}^{i} d\Omega = 0,$$

(16)

$$R_{M} = \int_{\Omega} \left[ \left( \rho \mathbf{u} \cdot \nabla \mathbf{u} \right) \phi^{i} - \nabla \cdot \left( -\mathbf{p} + \frac{\partial \mathbf{T}}{\partial t} \right) \phi^{i} \right] d\Omega = 0,$$

(17)

$$R_{E} = \int_{\Omega} \left( \rho C_{p} \mathbf{u} \cdot \nabla T - \kappa \nabla^{2} T - \nabla \cdot \left( \nabla T \right) \phi^{i} \right) d\Omega = 0,$$

(18)

By applying the divergence theorem in order to decrease the order of differentiation and to project the natural boundary conditions for heat flux and stress at the boundaries $\Gamma$ of the domain $\Omega$, Eqs. (17) and (18) reduce to:

$$R_{M} = \int_{\Omega} \left[ \left( \rho \mathbf{u} \cdot \nabla \mathbf{u} \right) \phi^{i} + \left( \frac{\partial \mathbf{T}}{\partial t} \right) \cdot \nabla \phi^{i} - \mathbf{n} \cdot \left( -\mathbf{p} + \frac{\partial \mathbf{T}}{\partial t} \right) \phi^{i} d\Gamma = 0,$$

(19)

$$R_{E} = \int_{\Omega} \left( \rho C_{p} \mathbf{u} \cdot \nabla T - \kappa \nabla^{2} T - \mathbf{n} \cdot \nabla T \right) \phi^{i} d\Gamma = 0.$$

(20)

Since essential boundary conditions (BCs) for $u$, $v$ and $T$ will be applied to all but the outflow boundary of the domain, Eqs. (19) and (20) will be replaced by these BCs. Consequently, the surface integrals in Eqs. (19) and (20) still need to be evaluated or replaced or handled in some way at the synthetic outflow. This is done here by applying the free boundary condition (FBC), which simply evaluates these integrals at each iteration at the outflow and thus finds the local values of the primitive variables $u$–$v$–$p$–$T$.

Our recent works [13,16] contain detailed derivations of the FEM formulation based on the “stiffness” matrix and “load” vector approach advocated by Huebner and Thornton [31]. This approach is better suited for Picard iterative schemes (direct substitution) [16] rather than Newton–Raphson schemes [1].

Some other features of the above formulation are as follows. No upwinding was found to be necessary for the energy equation in the range of the present non-isothermal simulations. The program uses a Newtonian (reference) “stiffness matrix” and puts all elastic stresses (or any non-linear viscous stresses) on the RHS “load vector”. In each 8-node quadrilateral element, the strain rates are interpolated with linear basis functions. Galerkin averaging is used on the strain rates to obtain a smooth field [30]. Then based on these strain rates, the viscoelastic stresses are calculated using a 15-point Gauss-Laguerre quadrature, which is very efficient for the calculation of stresses for any number of relaxation modes, since this is an additive procedure [24,25,30]. Furthermore, the code applies the Adaptive Viscoelastic Stress Splitting (AVSS) scheme for handling the viscoelastic stresses [33]. This basically means that the viscosity entering the “stiffness matrix” of element $e$ is a reference viscosity $\eta_{\text{ref}}$, which depends on the element size $h_{e}$.

![Fig. 3.](image3.jpg) Pressure-driven flow of a Newtonian fluid in a planar channel at a 45°-angle with the horizontal: (a) $u_{x}$-contours $U$, (b) $u_{y}$-contours $V$. Results by applying the zero-traction boundary conditions at outflow show that the flow does not develop properly to the exit.

![Fig. 4.](image4.jpg) Poiseuille flow in a tube. Boundary conditions and finite element grid ($5 \times 5$). FBC stands for the free boundary condition.
Fig. 5. Contours of field variables in Poiseuille flow of the integral upper-convected Maxwell (UCM) fluid: \( W_s = 1 \) and \( \theta = -0.25 \).

Fig. 6. Axial pressure distribution of the integral upper-convected Maxwell (UCM) fluid at \( W_s = 1 \): (a) \( \theta = 0 \), (b) \( \theta = -0.25 \).

Fig. 7. Schematic diagram of flow through a 4:1 contraction geometry and boundary conditions for the numerical simulation. In the isothermal case, either fully developed velocity profile or free boundary conditions (FBC) are used at the outflow boundary.
and the maximum component of the elastic stress tensor $\tau_{\text{el}}$ and the velocity vector $\bar{u}$, i.e.,

$$\left(\eta_{\text{ref}}\right)_e = \frac{h_{\text{ref}}}{\bar{u}_{\text{max}}}.$$

The AVSS is capable of providing accurate results for test problems (e.g., Poiseuille flow of a UCM fluid) for very high $W_s$ numbers (see below), which are impossible to obtain without it. The details of the method and its good solution characteristics are given explicitly in [33].

In the present work, the program was modified for implementing the FBC. The terms of the FBC are (axisymmetric geometry):

$$\mathbf{F} = \left\{ \begin{array}{l} F_r \\ F_z \end{array} \right\} = \int_{\Gamma_{\text{NC}}} \left( \bar{n} \cdot \left(-p^{\text{I}} + \bar{\tau}\right) \right) \phi d\Gamma = \int_{\Gamma_{\text{NC}}} \left( \frac{n_1}{n_1 + n_2} (-p + \tau_{rr} + \tau_{zz} + n_1 \tau_{\bar{u}r} - n_2 \tau_{\bar{u}z}) \phi \right) d\Gamma, \quad i = 1, 3$$

$$\mathbf{F}_q = \int_{\Gamma_{\text{NC}}} \left( \bar{n} \cdot k \nabla \bar{\tau} \right) \phi d\Gamma = \int_{\Gamma_{\text{NC}}} k \left( \frac{\partial \bar{T}}{\partial \bar{r}} + \frac{n_2}{n_1 + n_2} \frac{\partial \bar{T}}{\partial \bar{z}} \right) \phi d\Gamma, \quad i = 1, 3$$

In the above it should be noted that the stresses $\bar{\tau}$ are the addition of the elastic stresses given by the constitutive Eq. (4) and the viscous stresses given with a reference viscosity $\eta_{\text{ref}}$. Thus, the stresses appearing in Eq. (22) are:

$$\tau_{rr} = \tau_{rr,\text{el}} + 2\eta_{\text{ref}} \frac{\partial \bar{u}_r}{\partial \bar{r}}, \quad \tau_{zz} = \tau_{zz,\text{el}} + 2\eta_{\text{ref}} \frac{\partial \bar{u}_z}{\partial \bar{z}}, \quad \tau_{\bar{r}z} = \tau_{\bar{r}z,\text{el}} + \eta_{\text{ref}} \left( \frac{\partial \bar{u}_r}{\partial \bar{z}} + \frac{\partial \bar{u}_z}{\partial \bar{r}} \right).$$

Fig. 8. Meshes used in this study: (a) mesh1; (b) mesh2.

Fig. 9. Axial velocity profiles along the symmetry line in the isothermal upper-convected Maxwell (UCM) fluid simulation at $W_s = 6$. Comparison with previous results [10].

Fig. 10. Axial stress profiles along the $r = 1$ line in the isothermal upper-convected Maxwell (UCM) fluid simulation at $W_s = 6$. Comparison with previous results [10].
The addition of a reference viscous term is the standard way of handling integral constitutive equations and is essential for the stability of the numerical scheme [33].

Our experience with the term of Eq. (22) in parallel flows, where the a priori known to be zero terms were set to zero, gave good results in the absence of a second normal stress difference, $N_2$. However, this approach for $N_2 = 0$ needed the imposition of $\partial \bar{u}_y / \partial z = 0$, as found out by Dimakopoulos and Tsamopoulos [12]. But still it did not give the correct results for the Poiseuille flow test problem with the UCM model. The problem was solved by allowing all terms appearing in Eq. (22) to be present and find their correct values upon iteration. Special care must be taken to put the correct signs in each term. Due to the nature of the Picard scheme (linear convergence, hence slow), of course many iterations were needed to satisfy the convergence criteria (for both the norm-of-the-error and the norm-of-the-residuals $<10^{-4}$) depending on the problem. For example, for the Poiseuille flow test problem with the UCM model, about 100 iterations were needed to satisfy the convergence criteria. For the contraction problem with the UCM model, the iterations increased to the order of 1000 for the highest elasticity level.

Finally, regarding the inflow boundary conditions, for integral models we need information about the prior deformation history. By assuming a fully developed velocity profile, as done in all cases here, we solve the one-dimensional (1-D) problem for a given flow rate with the K-BKZ model, as it simplifies in steady simple shear flow. Also, the deformation tensor $D$ is known in steady simple shear flow, which is needed for starting the particle-tracking procedure. The 1-D problem is solved with 1-D finite elements employing quadratic basis functions for the velocity.

4. Results and discussion

4.1. Newtonian flow at an angle

We begin our numerical tests for a Newtonian fluid flowing under pressure in a planar channel making a $45^\circ$-angle with the horizontal as shown in Fig. 1. The choice of this simple problem is to show the power of the free boundary condition at the outflow, arbitrarily cut at a length equal to $H$ after turning, where $H$ is the channel gap. It also serves as a test for checking purposes by others, should they want to test FBC with their code. The boundary conditions are shown in Fig. 1. These involve a fully developed velocity profile at inflow $\mathbf{A}F$ ($u_x = Hv - y^2$ and $u_y = 0$) corresponding to an average velocity $U = 1$, and zero velocities at the solid walls $ABC$ and $FED$. At outflow $CD$ the usual practice is to put zero surface tractions $T = 0$, since the profile is not known there. The pressure is also set to zero at one node ($D$). Here, the other alternative is to apply the free boundary condition with no pressure set to zero at any point. This is essential when applying the FBC [13].

Fig. 2a shows the finite element grid used. It is a very sparse grid consisting only of 50 elements, the point being that the method, when correctly implemented, gives good results even for the sparsest of grids. The results employing the FBC are shown in Fig. 2 as velocity vectors (Fig. 2b), contours of the two velocity components $u_x = U$ and $u_y = V$ (Fig. 2c and d), streamlines STR (Fig. 2e), and isobars $P$ (Fig. 2f). The contours here and in the following are given as 11 equidistant lines between the minimum and maximum values (not shown). Thus, for the stream function $\psi$ the minimum value is 0 and the maximum value is 1, while the contour interval is $\Delta \psi = 1/12 = 0.0833$. The results show a nice smooth parallel flow to the channel walls all the way to the outlet, while the isobars are normal to the flow. Denser grids simply make the results smoother.

On the other hand, employing the zero-traction boundary condition at outflow gives the velocity contour results of Fig. 3, where it is aptly shown that they are not proper. Therefore, this example is another good manifestation of the efficiency of FBC applied in a flow at an angle cut at some arbitrary distance of the flow domain.

4.2. Poiseuille flow of a UCM fluid

We then tested the implementation of the FBC with the integral UCM fluid in simple pressure-driven (Poiseuille) flow in a tube. Fig. 4 shows the solution domain and boundary conditions, together with a $5 \times 5$ finite element grid in the same line of understanding as before, namely that if the method is correct it should work even with the sparsest of grids. Because of symmetry only one half of the flow domain is considered. The boundary conditions in this type of problem are: along the inlet DA a fully-developed velocity profile is given, $u_x = 1 - r^2$ and $u_y = 0$; along the symmetry line AB, $r \gamma = 0$, $u_y = 0$; along the die wall no slip conditions are imposed, $u_x = u_y = 0$; and along the outlet BC either a fully-developed profile is given, $u_x = 1 - r^2$ and $u_y = 0$ (and this is a necessity for viscoelastic fluids due to the presence of non-zero normal stresses),
or the FBC is prescribed. The pressure $P$ is set to 0 at point C or is left free when using the FBC [13,16].

The K-BKZ model reduces to the integral UCM fluid model with the choice of parameters mentioned in Section 2.1. For this case, there is an analytical solution available, which is the same for the explicit second-order fluid (SOF) model [16]. In cylindrical coordinates the solution is [33]:

$$u_z = 1 - r^2, \quad \tilde{\gamma} = -4Ur, \quad (\Delta P/L)_{r=0} = 8U, \quad (\Delta P/L)_{r=1} = 8U - \left(2\bar{\theta} - \frac{\bar{\theta}}{1-\bar{\theta}}\right)Ws^2,$$

$$\tau_{rz} = \frac{\bar{\theta}}{1-\bar{\theta}}Ws^2, \quad \tau_{rr} = \frac{\bar{\theta}}{1-\bar{\theta}}Ws^2, \quad \tau_{\theta\theta} = 0.$$

(25)

Thus, for an average velocity $U = 0.5$, it follows that $\tau_{rz} = \tilde{\gamma} = 2$; furthermore, if $Ws = 1$ and $\theta = -0.25$, it follows that the pressure drop at the centerline $\Delta P_{cl} = 4$, at the wall $\Delta P_w = 5.2$; and the stresses $\tau_{rz} = 3.2$, $\tau_{rr} = -0.8$, $|\tau| = \sqrt{\tau_{rz}^2 + \tau_{rr}^2 + \tau_{\theta\theta}^2} = 3.07$.

The results for $Ws = 1$ and $\theta = -0.25$ are given in Fig. 5 for the contours of various flow variables, which are the stream function $\psi$, the axial velocity $u_z$, the pressure $P$, the normal stresses $\tau_{rz}$ and $\tau_{rr}$, and the shear stress, $\tau_{\theta\theta}$. Eleven contours are drawn, equidistant between the maximum and minimum values. We observe that all contours (except the pressure) are perfectly parallel to the flow, as they should, since this is a fully-developed shear flow. The pressure contours (isobars) show the distinct curvature associated with a non-zero $N_2$. When $N_2 = 0$, the isobars are perfectly vertical. The pressure values have been recalculated by subtracting the pressure at the exit corner node (point C), so that the pressure becomes zero there.

**Fig. 6** shows the axial pressure distributions for $Ws = 1$ and $\theta = 0$ or $\theta = -0.25$. In both cases, the axial pressure distribution is linear. However, when $\theta = 0$, the axial pressure distributions along the wall and the centerline coincide. When $\theta \neq 0$, there is a radial distribution of pressure, which is quadratic in $r$, and the results between the wall and the centerline are different. In both cases, the numerical results agree exactly with the analytical solutions of Eq. (25) either by using the fully-developed profiles at exit or the FBC.

It is interesting to note that the upper limits for convergence were different for $\theta = 0$ and $\theta \neq 0$. In the former case, no upper limit was found even for $Ws = 10^6$, which is due to the use of AVSS [33]. In the latter case, an upper limit was found for $Ws = 2$ with $\theta = -0.25$. The same results were found by using explicit differential models in our previous work [16].

### 4.3. UCM isothermal contraction flow

We now continue with the isothermal UCM flow in the benchmark problem of a 4:1 abrupt axisymmetric contraction, which was studied before by Park and Lee [10]. **Fig. 7** shows the solution domain and boundary conditions. Because of symmetry only one half of the flow domain is considered, as was done in the previous works [10,20–22].

The simulations for the benchmark problem have been run with the FEM meshes shown in **Fig. 8**. These are similar to the meshes used by Park and Lee [10], having about the same number of elements and nodes. Park and Lee [10] have used the Newton–Raphson (N–R) scheme in their formulation together with the differential counterpart of the UCM fluid, but the results should be the same with the UCM integral model. As shown, many elements are concentrated near the die entry due to the singularity there, and at the outlet to make sure that the FBC is accurately calculated.
We present results at the highest elasticity level of $W_{S} = 6$ (more specifically, and by choosing $\lambda = 0.1 \, \text{s}$, this corresponds to a reduced average outlet velocity $U/R = 15$ or $\dot{\gamma}_{A} = 60 \, \text{s}^{-1}$). This is the first time we have used the K-BKZ model as UCM for such an elevated $W_{S}$ value. The trick here to get a converged solution at this level was to apply the adaptive viscoelastic stress-splitting (AVSS) [33] and increase slowly the viscoelastic stresses of Eq. (4) which enter the load vector by using severe under-relaxation with a factor $\omega_s = 0.01$. This required many Picard iterations (in the order of $10^{3}$), but the results were good and were validated by those obtained by Park and Lee [10] with the differential equivalent of UCM and using the streamline-upwind (SU) scheme for the integration of viscoelastic stresses.

Fig. 9 shows the axial distribution of the axial velocity at the centerline in comparison with the results by Park and Lee [10]. The agreement is good. The same can be also said for the normal stress $\tau_{zz}$ and shear stress $\tau_{rz}$ axial distributions along the $r = 1$ line, shown in Fig. 10a and b. The discrepancies shown can be attributed to different grids and integration schemes. This is more evident near the singularity, where oscillations are present with both methods, but these oscillations are local and do not affect the rest of the flow field. It should also be noted that the values from [10] have been read from the corresponding graphs by using a digitizing software.

In our previous work [16], we have also checked the non-isothermal Newtonian test by Park and Lee [10] with excellent results. Thus, the non-isothermal implementation of FBC has been tested before. We can therefore confidently say that the FBC has been correctly implemented for viscous and viscoelastic flows, with or without thermal effects. For this reason we do not present here the results for the non-isothermal UCM model, which does not add any more value to the already obtained results. Instead, we proceed with the K-BKZ model for the IUPAC-LDPE (sample A) melt, which represents a real-case polymer melt flow.

4.4. K-BKZ isothermal contraction flow

The isothermal results for a 4:1 axisymmetric contraction for the IUPAC-LDPE melt have been presented before [34]. Here, we repeat the simulations first for the isothermal case but with the FBC.
implemented. Then we embark upon the non-isothermal simulations with the FBC.

Results are shown for a test run at $\gamma_0 = 80 \text{ s}^{-1}$. At this elevated apparent shear rate, the fully-developed wall shear rates in the die are about $120 \text{ s}^{-1}$. The Weissenberg number is $W_s = \frac{\gamma_0}{\lambda} = 4700$, a highly elevated value due to the very long average relaxation time. A better measure for the elasticity of the melt is the stress ratio $S_R = \frac{\eta_0}{\eta_L}$ for the pressure distributions along the walls as shown in Fig. 11b. The pressures for $L/R = 10$ have been shifted to coincide with the ones at $L/R = 20$. It is again noted that no zero reference pressure is set anywhere in the flow field when implementing the FBC. The results for the pressure are given in MPa due to the real data used in the simulations.

We observe an excellent agreement from the two domains, meaning that the FBC can be safely used in truncated domains with this type of viscoelastic fluids. Thus, we can confidently say that the FBC has been correctly implemented for viscoelastic flows with integral constitutive equations including a non-zero second normal stress difference ($\theta = -0.25$) in complex domains. It is worth mentioning here that truncating the domain to $L/R = 5$ made the convergence much slower and more difficult for elevated flow rates.

The streamlines and isobars from the simulations are given in Fig. 12a and b. The pressure values are divided by $\eta_0 = 51,064 \text{ Pa s}$.

The salient features of this flow are the existence of a vortex in the reservoir (also found in [34]) and the parabolic contours of the pressure in the die due to a non-zero $\theta$-value (cf. Fig. 6). The values $\theta = 0$ and $\theta = -0.25$ did not change in any visible way the streamline patterns, while the pressures were affected more, as shown in Fig. 12c, where for $\theta = 0$ the isobars are now vertical lines in the die.

### 4.5. K-BKZ non-isothermal contraction flow

The LDPE melt has a temperature-dependent viscosity according to the Arrhenius relationship (Eq. (8)). The thermal data for the LDPE melt are given in Table 2. Under these conditions and at $\gamma_0 = 80 \text{ s}^{-1}$, the Peclet number was $Pe = 16,256$ and the Nahme number was $Na = 14.87$. The maximum temperature rise $\Delta T_{\text{max}}$ under these conditions reached $7.7^\circ \text{C}$ for the longer die with $L/R = 20$.

The boundary condition at the outlet is only the FBC either for $L/R = 10$ or 20. A denser grid was necessary in the non-isothermal viscoelastic simulations, having more cuts near the outflow for good results in the longer domain ($L/R = 20$). All non-isothermal results are obtained with $\theta = -0.25$. Again, truncating the domain to $L/R = 5$ made the convergence much slower and more difficult for elevated flow rates.

We present results first for the axial velocity and pressure distributions in Fig. 13. The velocity distributions are along the centerline while those for the pressure are along the wall. In both cases the truncated domain at $L/R = 10$ gave the same results as those from the long domain with $L/R = 20$ up to 10R. Temperature results are given in Fig. 14. In particular, Fig. 14a shows the centerline axial temperature rise, which is minimal due to the very high convection ($Pe$ number), hardly rising a fraction of a degree. Both domains give identical results in the common length of 10R.

Fig. 14b shows the radial temperature profile at $z = 10R$ either
using a truncated domain with \( L/R = 10 \) or 20. The results coincide. The maximum temperature rise is close to the walls and is about 5 °C higher than the wall temperature of 150 °C at \( L/R = 10 \). When using a longer domain with \( L/R = 20 \), the maximum temperature rise is higher (about 7.7 °C) as expected.

Fig. 15 shows streamlines, isobars and isotherms obtained from the K-BKZ non-isothermal flow simulations. The pressure values are divided by \( \eta_0 = 51,064 \text{ Pa s} \). The vortex results are not affected in a visible way by the non-isothermal simulations. The same can also be said for the pressures, where the isobars have been given in MPa. The curved isobars reflect the presence of a non-zero second normal stress difference \( N_2 \). Finally, the isotherms show that the temperature rises towards the exit and near the walls, where the thermal boundary layers developed due to viscous dissipation effects that are convected downstream by the flow. All results at the outflow are well behaved, so we can confidently say that the FBC has been implemented correctly and works well for non-isothermal viscoelastic flows governed by integral models.

5. Conclusions

We have implemented the free (open) boundary condition to viscoelastic non-isothermal flows in the context of integral constitutive equations of the K-BKZ type. A non-zero second normal stress difference has been correctly implemented without needing ad hoc zeroing out of terms [12]. Code validation was carried out against analytical results and against previous results by Park and Lee [10] in the benchmark problem of a 4:1 axisymmetric contraction. First Newtonian isothermal flows at an angle were successfully tested in arbitrarily truncated domains. Then, the Poiseuille flow of the integral upper-convected Maxwell (UCM) fluid was successfully tested, as well as strong viscoelastic isothermal flows of the UCM at Weissenberg number \( W_0 = 6 \) in the 4:1 contraction [10].

Finally, the FBC was tested with the K-BKZ model used for fitting rheological data for the IUPAC-LDPE melt, including a non-zero second normal stress difference. For elevated apparent shear rates, a truncated domain (\( L/R = 10 \)) gave identical results for the velocities, pressures and temperatures as a longer domain (\( L/R = 20 \)), thus showing the usefulness of the FBC in viscoelastic flows. This is particularly true at elevated values of the apparent shear rate, where very long domains are needed to fully relax the stresses and impose fully-developed conditions at the outlet. The FBC is particularly suited for strong viscoelastic flows, due to the highly convective nature of these flows, regarding the stresses and their hyperbolic character.

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