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THREE-DIMENSIONAL EXTRUDATE SWELL: FORMULATION WITH THE STREAM TUBE METHOD AND NUMERICAL RESULTS FOR A NEWTONIAN FLUID

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SUMMARY

Stream tube analysis, already applied to two-dimensional extrudate swell problems involving rate and integral constitutive equations for incompressible fluids, is now considered in the problem of free surface determination in a three-dimensional flow situation. The method allows computation of the unknown free surface by considering only a 'peripheral stream tube' limited by the wall and the jet surface and an inner stream surface. Those boundary surfaces are determined by considering the conservation equations together with boundary condition equations, solved by the Levenberg/Marquatdt optimization algorithm. The method leads to a considerable reduction in the number of degrees of freedom and the storage area. As in a previous study in the two-dimensional case, singularity problems in the vicinity of the junction points between the wall and the free surface are avoided. However, the numerical method still allows evaluation of stress peaks due to the singularity at the exit, as may be observed for results obtained with a Newtonian fluid in a duct of square cross-section.

KEY WORDS: 3D extrudate swell; free surface flow; stream tube method; Levenberg–Marquardt algorithm

1. INTRODUCTION

Significant advances were made in numerical simulations of three-dimensional extrudate swell problems at the end of the 1980s. They notably involved the works presented by Bush and Phan-Thien,[1] Tran-Cong and Phan-Thien,[2,3] Karagiannis *et al.*,[4] Shiojima and Shimazaki,[5] Wambersie and Crochet[6] and Legat and Marchal.[7,8] In relation to complex geometries of 3D flow situations, the authors adopted finite element methods to compute the relevant unknowns of the problem, namely velocity components (u, v, w) and pressure p, leading to a great number of degrees of freedom. On one hand, purely viscous constitutive equations were generally considered in flow simulations of extrudate swell. On the other hand, 3D numerical flow simulations using memory-integral constitutive equations still remain a difficult task, since the flow path lines are not planar curves. This produces a very delicate particle tracking problem, since streamlines do not pass through mesh points.

The stream tube method, introduced some years ago,[9,10] allows flow computation by means of an unknown transformation T, assumed to be one-to-one, between a physical flow domain D and its mapped domain D^*, used as computational domain, in which transformed streamlines are parallel and straight. Conditions for application of stream tube analysis have been considered in several papers[10,11] and have also concerned flow situations with recirculations.[12] Since extrudate swell flow

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involves only open streamlines, a one-to-one transformation may be defined, leading to no restriction in applying stream tube analysis. Previous studies of two-dimensional swell flows with this method were carried out for differential13 and integral[14] constitutive equations. Before considering the numerical approach related to the three-dimensional flow problem, we find it of interest to summarize the main features of the stream tube method as follows.

(i) Mass conservation is automatically verified by the formulation. In contrast with classical methods, the primary unknowns of the problem are the pressure and one or two mapping functions (f or f and g) in the two-or three-dimensional case respectively.
(ii) In 2D and 3D situations a very simple mesh may be built in the computational domain on the rectilinear mapped streamlines, leading to the definition of simple discretization schemes for solving the equations. The differential and integral operators which may be involved in viscoelastic constitutive equations may be easily taken into account.[11,13]
(iii) The flow may be computed by considering successive subdomains of D, the stream tubes, from the wall to the central region, provided that the action of the complementary flow domain is taken into account. This property is to be emphasized in the case of the swelling flow problem, for which only consideration of the 'peripheral stream tube' involving the wall and the free surface permits determination of the unknown jet surface. Thus a reduction in the number of unknowns, leading to a significant shortening of computing time and storage memory, is expected when solving the relevant equations.

In the present work concerned with the application of the stream tube method to numerical simulation of three-dimensional extrudate swell flows, only the purely viscous case is studied initially. Similarly to a recent study of two-dimensional swell problems,[13] the analysis presented here avoids considering explicitly the singularity problems in the vicinity of the junction points between the wall and the free surface. However, the calculations performed in the present work still enable the singularity effects at the exit section z_0 to be emphasized. The flow relates to the case of a die of constant cross-section along the z-axis, the duct length being considered as large enough to assume fully developed flow at sections $z \leqslant z_1$. The flow domain is defined such that $z_1 \leqslant z \leqslant z_2$. The section z_2 starts the solid flow region in the free jet (Figure 1).

Section 2 of the paper presents the basic elements of the stream tube method in relation to the three-dimensional free jet problem. In Section 3 we examine the approximating schemes presented for computing the unknowns. In Section 4 the governing equations are written, with the aim of considering the peripheral stream tube, limited inside by an inner stream surface of the physical domain and outside by the wall and the unknown free surface to be calculated. The criterion for

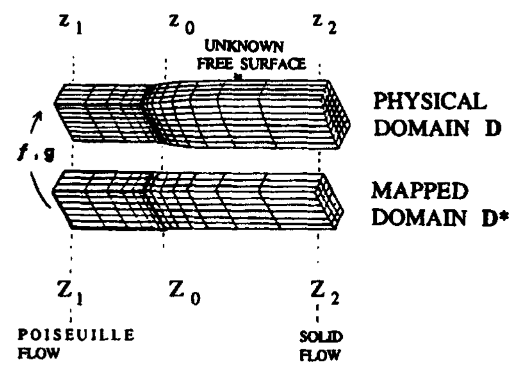

Figure 1. Physical and mapped domains in three-dimensional extrudate swell problem

determination of the jet surface is also examined. Section 5 presents the numerical procedure and swell results, obtained by using only the peripheral stream tube, for a Newtonian constitutive equation corresponding to the flow of a fluid emerging from a duct of square cross-section. Concluding remarks are given in Section 6.

2. THE STREAM TUBE METHOD IN THREE-DIMENSIONAL EXTRUDATE SWELL PROBLEMS

The physical and mapped domains D and D^* corresponding to the transformation T: $D \rightarrow D*$ are illustrated by the example of Figure 1. Cylindrical co-ordinates (r, θ, z) are used in the flow domain D. The mapped domain $D*$ is defined as a straight cylinder whose basis is identical with the upstream cross-section A_0 of the physical flow domain D at $z = z_1$. This section limits the fully developed flow region where the kinematics are known. The domains D and $D*$ are related to the equations

$$r = f(R, \Theta, Z), \qquad \theta = \mathsf{g}(R, \Theta, Z), \qquad z = Z. \tag{1}$$

Here f and g denote the mapping functions related to T, to be determined numerically, and (R, θ, Z) are the cylindrical co-ordinates associated with the transformed domain $D*$ where mapped streamlines are rectilinear and parallel to the z-axis. At section z_1 the relations

$$r = R = f(R, \varphi, z = z_1), \qquad \theta = \varphi = \mathsf{g}(R, \varphi, z = z_1), \qquad z_1 = Z_1 \tag{2}$$

may easily be verified. From a geometrical viewpoint the mapping function f may be considered as a stream surface limiting a stream tube. Thus a streamline $\mathscr{L}$ is defined by the intersection of a stream surface f and a surface g. By using cylindrical co-ordinates, it is possible to consider variations in the function g to be related to the 'warping' of the streamline curves, as illustrated in Figure 2. A plane flow situation is to be related to the case $\theta = \varphi$.

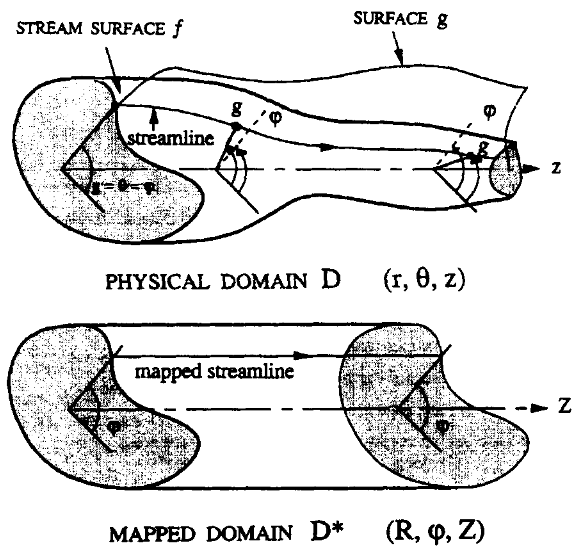

Figure 2. Streamline curves in respective physical and mapped domains D and D^* in streamtube analysis

The velocity vector $\mathbf{V}$ in cylindrical co-ordinates (r, θ, z) is given by

$$\mathbf{V} = u(r, \theta, z)\mathbf{c}_r + v(r, \theta, z)\mathbf{c}_\theta + w(r, \theta, z)\mathbf{c}_z \tag{3}$$

and is known at the upstream section z_1, by analytical or numerical means (see e.g. Reference 15), for a Newtonian fluid. Here $(\mathbf{c}_r, \mathbf{c}_\theta, \mathbf{c}_z)$ denotes the orthonormal frame related to the cylindrical co-ordinates. At the upstream Poiseuille flow section to the tube $(z = z_1)$ and the solid jet flow section $(z = z_2)$ the velocity vector is assumed to be written as

$$\mathbf{V} = w(r, \theta, z_1)\mathbf{c}_z \quad \text{at } z = z_1, \qquad \mathbf{V} = w_2\mathbf{c}_z \quad \text{at } z = z_2. \tag{4}$$

where w_2 denotes the solid flow velocity.

The description of incompressible 3D flows by stream tube analysis has already been formulated in a previous paper[11] for confined ducts involving a circular upstream section. For a simply connected duct of general shape we may introduce a function $\Psi(r, \theta)$ at section z_1 via the relationship

$$w(r, \theta, z_1) = \Psi(r, \theta)/r, \quad r \neq 0. \tag{5}$$

Using the boundary condition equations (2), we still adopted the same notation for in order to consider, in terms of variables (R, φ, Z), a function related to a similar equation to equation (5), as

$$w(R, \varphi, Z_1) = \Psi(R, \varphi)/R, \quad R \neq 0. \tag{6}$$

Hence it may be shown that the velocity components are given by

$$u = f'_Z\Psi(R, \varphi)/(f\Delta), \qquad v = g'_Z\Psi(R, \varphi)/\Delta, \qquad w = \Psi(R, \varphi)/(f\Delta). \tag{7}$$

In equations (7), Δ denotes the Jacobian, assumed to be non-singular, of the transformation T:

$$\Delta = |\partial(r, \theta, z)/\partial(R, \varphi, Z)| = f'_R g'_\varphi - f'_\varphi g'_R. \tag{8}$$

The relations

$$\Gamma = f'_\varphi g'_R - f'_Z g'_\varphi, \qquad \Sigma = f'_Z g'_R - f'_R g'_Z \tag{9}$$

are also considered in order to simplify the writing of the equations. Derivative operators relating the sets of variables (r, θ, z) and (R, φ, Z) may be written as

$$\begin{aligned} &\partial/\partial r = (g'_\varphi \partial/\partial R - g'_R \partial/\partial\varphi]/\Delta, \qquad \partial/\partial\theta = [-f'_\varphi \partial/\partial R + f'_R \partial/\partial\varphi]/\Delta, \\ &\partial/\partial z = (\Gamma\partial/\partial R + \Sigma\partial/\partial\varphi)/\Delta + \partial/\partial Z. \end{aligned} \tag{10}$$

In this approach we consider stream surface f where cross-sections at z_1 define contour values of the velocity component w ($w =$ constant). Consequently, for simple connected ducts the stream tubes (related to the mapping function f to be determined) involved in the present flow analysis are limited at the upstream section z_1 by contour values such that the zero-velocity contour curve corresponds to the wall when assuming the no-slip velocity condition. It should be pointed out that in contrast with two-dimensional flow situations, where the positions of streamlines at the solid flow sections z_2 are determined by conservation of flow rate, the corresponding positions of a streamline stream at the solid flow section z_2 are unknown in three-dimensional cases. Figure 3 illustrates the respective cross-sections of stream tubes related to contour values of the non-zero component w for the Poiseuille flow of a Newtonian fluid in a duct of rectangular cross-section $(z = z_1)$ and those related to the solid flow velocity at $z = z_2$.

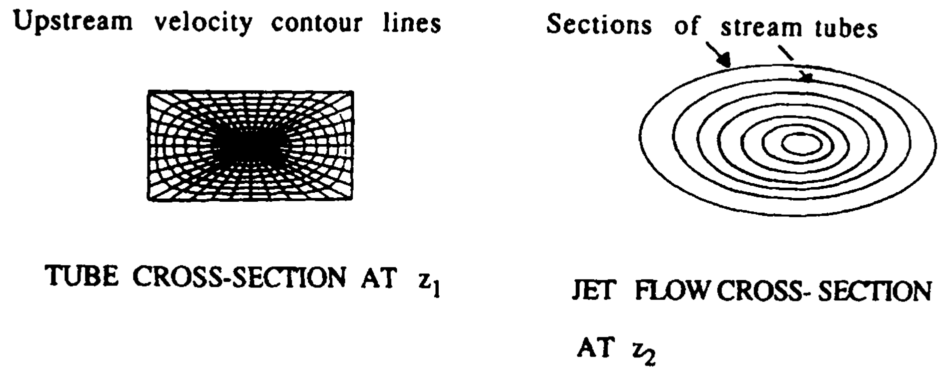

Figure 3. Upstream and downstream cross-sections of streamtubes for three-dimensional extrudate swell problem

3. STREAMLINE APPROXIMATION—DISCRETIZATION OF UNKNOWNS

To approximate the jet surface in a two-dimensional extrudate swell problem. Batchelor and Horsfall[16] proposed the following one-dimensional equation to describe the free surface in a meridian plane:

$$R(z) = r_0 + A\{1 - \exp[-B(z - z_0)]\}. \tag{11}$$

In this equation, A and B are constants and r_0 denotes the free surface co-ordinate at the exit section $z = Z = z_0$. The above relation, also considered e.g. in Reference 17, was proved to fit well with experimental data relating to swell of various polymer solutions and melts. Starting from equation (11), a generalization by the authors of this paper[13,14] to approximate streamlines in the total flow domain, from the Poiseuille flow section $z = z_0$ to the solid flow section $z = z_2$ of the free jet, was also found to be consistent for streamlines in two-dimensional extrudate swell problems.

In 3D situations we still adopt approximate functions derived from the two-dimensional relations proposed in References 13 and 14 to relate stream surfaces f defined in the basic equations (1). Accordingly, the mapped function f may be written as a function involving the azimuth angle φ such that

$$f(R, \varphi, Z) = C_1(R, \varphi, Z) + A(R, \varphi), q(Z)\{1 - \exp[-(Z - Z_0)B(\varphi, Z)]\} \tag{12}$$

in the tube for $Z_1 \leqslant Z \leqslant Z_0$. In the jet for $Z_0 \leqslant Z \leqslant Z_2$ we assume the equation

$$f(R, \varphi, Z) = f(R, \varphi, Z_2) - A(R, \varphi) \exp[-(Z - Z_0)B(\varphi, Z)]\}. \tag{13}$$

The functions $q(Z)$ and $C_1(R, \varphi, Z)$ have the same meanings as in the two-dimensional case[13,14] and continuity of the equations for f is verified at junction points of abscissa Z_0. Streamline warping curves $\mathfrak{L}$ belong to stream surfaces $f(R, \varphi, Z)$. The function g, which must satisfy the boundary condition (2), is to be computed by point values on the three-dimensional mesh defined in the mapped domain $D*$, related to the peripheral stream tube which involves the wall and the unknown free surface.

For the purposes of illustration and understanding of the different quantities involved in equations (12 and 13), which are mostly related to geometrical considerations, Figure 4 shows flattened views of the peripheral stream tube $\mathscr{B}$ in the physical flow domain D and of its mapped domain in $D*$ for a rectangular duct. The stream tube is limited outside by the boundary surface $\mathscr{S}_0$ involving the wall $\mathscr{W}_0$ and the free surface Σ_0 and inside by a stream surface f_3 or $\mathscr{S}_3$) close to the surface $\mathscr{S}_0$. As may

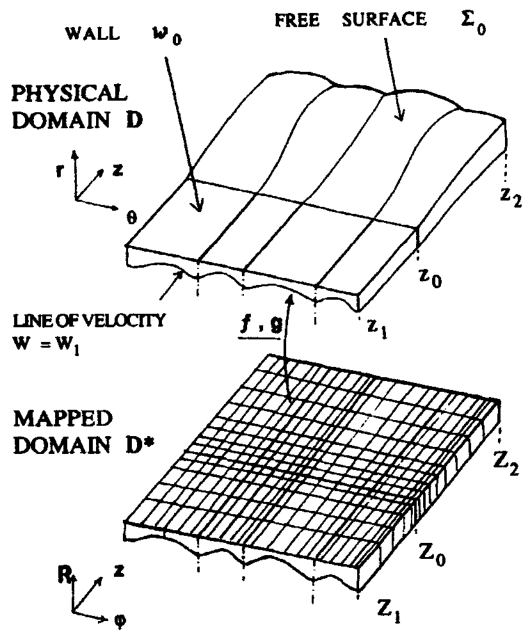

Figure 4. Flattned views of peripheral stream tube in physical domain D and of its transformed domain in mapped computational domain D^*

be expected, the surfaces $\mathscr{S}_0$ and $\mathscr{S}_3$ of the stream tube $\mathscr{B}$ are not generally plane. For the mapped stream tube $\mathscr{B}*$, $R_0(\varphi Z)$ are used to denote variables related to the outer and inner boundary stream surfaces $\mathscr{S}_0$ and $\mathscr{S}_3$ respectively. These surfaces are close enough to ensure that the quantities $\| R_0(\varphi, Z) - R_3(\varphi, Z) \|$ are small. Thus, given a section Z of the flow domain, the mapped peripheral stream tube $\mathscr{B}*$ in domain $D*$ may be defined by the variables (R, φ) such that

$$\varphi_0 \leqslant \varphi \leqslant \varphi_1, \qquad R_2(\varphi, Z) \leqslant R \leqslant R_0(\varphi, Z). \tag{14}$$

In equation (14), φ_0 and φ_1 denote the limit values of the azimuth angle φ, the maximum difference $\varphi_1 - \varphi_0$ being equal to 2π when the duct involves no symmetry.

According to these considerations, the functions A and B may be approximated as

$$A(R, \varphi) = \alpha_0(\varphi) + \alpha_1(\varphi)[R - R_0(\varphi)] + \mathcal{O}([R - R_0(\varphi)]^2), \tag{15}$$

$$B(R, \varphi) = \beta_0(\varphi) + \beta_1(\varphi)[R - R_0(\varphi)] + \mathcal{O}([R - R_0(\varphi)]^2). \tag{16}$$

Similarly, the mapping function g is expressed in the peripheral stream tube by the equation

$$g(R, \varphi, Z) = \gamma_0(\varphi, Z) + \gamma_1(\varphi, Z)[R - R_0(\varphi, Z)] + \mathcal{O}([R - R_0(\varphi, Z)]^2). \tag{17}$$

The functions $\alpha_0(\varphi)$, $\alpha_1(\varphi)$, $\beta_0(\varphi)$, $\beta_1(\varphi)$, $\gamma_0(\varphi, Z)$ and $\gamma_1(\varphi, Z)$ of equations (15)–(17) are to be determined numerically from the relevant equations of the swell problem.

4. GOVERNING EQUATIONS—SWELLING CRITERION

4.1. *Governing equations in peripheral stream tube $\mathscr{B}$*

The equations to be written in the swell problem are considered under isothermal conditions, with restriction to flow in the peripheral stream tube. Surface tension, inertia and body forces are ignored and no traction on the jet at section z_2 is assumed. These assumptions may be considered as good for extrusion flows of high-viscosity fluids. The governing equations involve the classical laws of conservation and are expressed in terms of the pressure p and unknowns related to mapping functions f and g.

(a) Mass conservation is automatically verified from the stream tube analysis, as already pointed out.

(b) Taking into account the previous assumptions, the classical dynamic equations may be written as

$$-\partial p/\partial r + \partial T^{rr}/\partial r + (1/r)\partial T_{r\theta}/\partial\theta + \partial T^{rz}/\partial z + (T^{rr} - T^{\theta\theta})/\partial r = 0, \tag{18}$$

$$-(1/r)\partial p/\partial\theta + \partial T^{r\theta}/\partial r + (1/r)\partial T^{\theta\theta}/\partial\theta + \partial T^{\theta z}/\partial z + 2T^{r\theta}/r = 0, \tag{19}$$

$$-\partial p/\partial z + \partial T^{rz}/\partial r + (1/r)\partial T^{\theta z}/\partial\theta + \partial T^{rz}/\partial z + T^{rz}/r = 0. \tag{20}$$

The use of variables (R, φ, Z) of the mapped domain $D*$ and derivative operators defined by equations (10) together with approximating relations for the mapping functions f and g leads to equations (18)–(20) being expressed in terms of the pressure gradient components as

$$\mathscr{A}_1\partial p/\partial R + \mathscr{B}_1\partial p/\partial\varphi = \mathscr{E}_1, \tag{21}$$

$$\mathscr{A}_2\partial p/\partial R + \mathscr{B}_2\partial p/\partial\varphi = \mathscr{E}_2, \tag{22}$$

$$\mathscr{A}_3\partial p/\partial R + \mathscr{B}_3\partial p/\partial\varphi + \mathscr{C}_3\partial p/\partial\varphi = \mathscr{E}_3. \tag{23}$$

In these equations, $\mathscr{A}_1, \mathscr{B}_1, \mathscr{A}_2, \mathscr{B}^2, \mathscr{A}_3, \mathscr{B}_3, \mathscr{C}_3, \mathscr{E}_1, \mathscr{E}^2$ and $\mathscr{E}^3$ denote functions of $\{f, \mathsf{g}, T^{ij}\}$. When expressing the stress components T^{ij} in terms of mapping functions f and g, these coefficients are functions of the unknowns $\{\alpha_0(\varphi), \alpha_1, (\varphi), \beta_0(\varphi), \beta_1(\varphi), \gamma_0(\varphi, Z), \gamma_1(\varphi, Z)\}$ defined by equations (15)–(17). Relations (21)–(23) are written on rectilinear streamlines L^* of the mapped computational domain $D*$. Thus the pressure p, assumed to be zero at the solid flow section z_2, may be determined by integration using the relation

$$p(R, \varphi, Z) = \int_{z_2}^{Z} \mathfrak{H}(R, \varphi, \zeta)\, \mathrm{d}\zeta, \tag{24}$$

where the integrand $\mathfrak{H}(R, \varphi, \zeta)$ is evaluated from equations (21)–(23).

(c) In stream tube analysis the equations may be solved on successive stream tubes provided that the action of the complementary flow domain is taken into account (see e.g. Reference 10). This condition may be expressed in 3D flows by the following equations related to the resultant and moment vectors $\mathfrak{R}$ and $\mathfrak{M}_0$:[11]

$$\mathfrak{R} = \int_{\partial\Omega} \sigma\mathbf{n}\, \mathrm{d}s = \int_{\partial\Omega} (-p\mathbb{I} + \mathbb{T})\mathbf{n}\, \mathrm{d}s = \mathbf{0},$$
$$\mathfrak{M}_0 = \int_{\partial\Omega} \mathbf{OM} \wedge \sigma(\mathbf{M})\, \mathrm{d}s = \mathbf{0}. \tag{25}$$

In equations (25), $\partial\Omega$ denotes the surface limiting the domain under consideration. Using the basic equations (1), the components of $\mathbf{n}$, the outward unit vector normal to the surface $\partial\Omega$, may be determined from a normal vector $\mathbf{N}$ to the surface given by

$$\mathbf{N}(g'_\varphi + g'_R f'_\varphi, -(f'_\varphi + f'_R f'_\varphi)/f, \Gamma - f'_\varphi \Sigma), \tag{26}$$

where Γ and Σ are defined by equations (9). When applied to the complementary flow domain of a stream tube and projected onto the three co-ordinate axes, relations (24) provide non-linear boundary condition equations to be considered together with the momentum conservation equations for the stream tube. It can be shown[11] that for ducts involving symmetries with respect to the z-axis, equations (22) reduce to the single scalar equation

$$\left(\int_{\partial\Omega} \sigma\mathbf{n}\, ds\right) \cdot \mathbf{c}_z = \left(\int_{\partial\Omega} (-p\mathbb{I} + \mathbb{T})\mathbf{n}\, ds\right) \cdot \mathbf{c}_z = 0. \tag{27}$$

(d) For the constitutive equation related to a Newtonian fluid the stress tensor is given by

$$\mathbb{T} = 2\eta_0 \mathbb{D} \tag{28}$$

(where η_0 is the fluid viscosity and $\mathbb{D}$ is the rate-of-strain tensor), the components of which, written in terms of mapping functions f and g, are replaced in equations (21)–(23).

The set of governing equations must be considered together with the classical 'simple' boundary condition equations in terms of the unknowns related to the mapping functions f and g.

4.2. *Procedure for determining unknown swell surface*

In this work the procedure for determining the free jet presents several similarities to that already adopted for two-dimensional swell studies with stream tube analysis[12,14] restricted to a peripheral stream tube. The criterion for determining the unknown swell surface Σ_0 in a three-dimensional extrudate swell is expressed by the two conditions

$$(\mathscr{C}_1) \quad I_1 = \int_{\partial\mathscr{B}} |(-p\mathbb{I} + \mathbb{T})_{\mathbf{n}}|\, ds = 0, \tag{29}$$

$$(\mathscr{C}_2) \quad [\mathbf{I}_2] = [\mathfrak{R} = \int_{\partial\mathscr{B}_c} (-p\mathbb{I} + \mathbb{T})\mathbf{n}\, ds; \mathfrak{M} = \int_{\partial\mathscr{B}_c} \mathbf{OM} \wedge \sigma(\mathbf{M})\, ds] \equiv [\mathbf{0}; \mathbf{0}]. \tag{30}$$

Equation (30) is related to the action of the complementary domain $\mathscr{B}_c$ of the peripheral stream tube $\mathscr{B}$ (given by equation (23)) limited by the upstream and downstream sections z_1 and z_2 respectively

Equations (29) and (30) require evaluation of the following quantities:

(i) the components of unit vectors $\mathbf{n}$ normal to the surfaces of the domains under consideration (equation (26))
(ii) the pressure p
(iii) the stress components T^{ij} at limit sections $z = z_1$ and $z = z_2$ and for points belonging to the inner lateral surface which limits the peripheral stream tube $\mathscr{B}$.

The pressure p and the stress components T^{ij}, unknown at points $\mathbf{M}_0$ of the boundary surface $\mathscr{S}^0$ (wall and free surface), are determined from the corresponding values of p and $\mathbb{T}$ on an internal stream surface $\mathbf{S}$ of the stream tube $\mathscr{B}$ using equation

$$\mathscr{E}(\mathbf{M}_0) \approx \mathscr{E}(\mathbf{M}) + (R_0 - R)\partial\mathscr{E}/\partial R|_{\mathbf{M}} + \mathscr{O}((R_0 - R)^2), \tag{31}$$

given φ and Z, the points $\mathbf{M}_0$ and $\mathbf{M}$ belonging to surfaces $\mathcal{S}^0$ and $\mathcal{S}$ respectively. This first-order approximation requires the quantity $\| R_0(\varphi, Z) - R(\varphi, Z) \|$ to be small for all sets (φ, Z) related to the mapped peripheral stream tube. In equation (31), $\mathcal{E}(\mathbf{M}_0)$ and $\mathcal{E}(\mathbf{M})$ denote functions evaluated at points $\mathbf{M}_0(R, \varphi, Z)$ and $\mathbf{M}(R, \varphi, Z)$ of stream tube $\mathcal{B}$ respectively.

For ducts involving symmetries, such as straight cylinders of regular polygonal cross-sections, the constraint (30) may be reduced to the scalar equation[11]

$$(\mathscr{C}^2) \quad I_2 = \left(\int_{\partial \mathcal{B}_c} (-p\mathbb{I} + \mathbb{T})\mathbf{n} \, \mathrm{d}s \right) \cdot \mathbf{c}_z = 0. \tag{32}$$

Equations (29) and (32) are to be considered together with the governing equations in the peripheral stream tube $\mathcal{B}$.

To approximate the spatial derivatives involved in the governing equations, the 'three-point formula' was used for derivatives in terms of R, Z and φ. According to this formula, given a function $Y(x)$ at three points X_1, x_2 and x_3, with respective corresponding values Y_1, Y_2 and Y_3, the x-derivative at x_1 is approximated by

$$[\mathrm{d}Y/\mathrm{d}x]_{x_1} \approx [Y(x_1) - Y(x_2)]/(x_1 - x_2) - [Y(x_2) - Y(x_3)]/(x_2 - x_3) + [Y(x_1) - Y(x_3)]/(x_1 - x_3). \tag{33}$$

The use of equation (33) in the mapped peripheral stream tube $\mathcal{B}*$ led to consideration in that subdomain of two stream surfaces $\mathcal{S}_1$ and $_2$ together with the outer stream surface $\mathcal{S}_0$ (transform of wall and free surface) and the limiting inner surface $\mathcal{S}_3$ (transform of wall and free surface) and the limiting inner surface $\mathcal{S}_3$.

5. NUMERICAL PROCEDURE AND SWELL RESULTS FOR EXTRUSION FROM A SQUARE DIE

5.1. Numerical procedure for solving equations

When using the governing equations in a peripheral stream tube to determine the unknown surface, it is of interest to underline several advantages of the proposed scheme.

(i) In contrast with classical methods of flow simulation, the mesh used for swell computations remains unchanged during the iterative process.
(ii) A new free surface does not have to be updated in order to check whether or not condition (32) corresponds to a minimum: the unknown swell surface is determined by *direct computation* of the unknowns, since this equation is involved in the overall set of governing equations. This possibility simplifies the numeral process in comparison with previous approaches with stream tube analysis.

Computational procedures are generally defined in such a way that the discretized governing equations of the problem are written as a closed set of equations. The use of stream tube analysis on a sub domain, as considered in the present study, leads to mathematical constraints being taken into account together with the relevant equations. The approximating schemes adopted for the streamlines are defined such that the numbers of equations and unknowns are different. As previously in two-dimensional studies of the extrudate swell problem[13] and others involving computation on successive stream tubes,[10,12] optimization methods such as the Levenberg–Marquardt algorithm are used (see e.g. References 18 and 19). This computational approach has proved its robustness and efficiency for such problems in relation to the significant sensitivity of the equations to changes in the mapping functions f and $\mathbf{g}$. This iterative procedure[19] allows a solution $\mathbf{X}*$ of the governing equations to be computed by a combination of two algorithms:

(i) the Newton algorithm, which converges quadratically but requires a good initial estimate $\mathbf{X}_{[0]}$ of the solution
(ii) the gradient algorithm, which has a linear convergence but converges for a less accurate initial estimate.

Although optimization methods may be time-consuming when the gradient and Hessian of the objective function defined in the minimization problem are to be evaluated, the Levenberg–Marquardt iterative algorithm[19] has proved to be efficient also in terms of computing time for solving the governing equations in the subregion $\mathscr{B}*$ of the computational domain.

5.2. *Numerical tests and results*

The steps in our calculations with the 3D code using the Newtonian equation concerned firstly the extrudate swell problem related to an axisymmetric duct and secondly the extrusion case related to a die of square cross-section with sides of length $2a$.

5.2.1. 3D tests for axisymmetric case. In order to test the basic numerical scheme, the problem of determining the swell surface of a free jet emerging from an axisymmetric duct of radius r_0 was examined. A peripheral stream tube consisting of an annular axisymmetric cylinder in the mapped domain was therefore considered. The tube and jet lengths adopted in our computations were defined as

$$(z_1 - z_0)/r_0 = -4, \qquad (z_2 - z_0)/r_0 = 10. \tag{34}$$

Taking into account the symmetry and periodicity properties of the duct geometry, a subdomain limited by planes $\theta = \mathbf{g} = \varphi = 0$ and $\theta = \mathbf{g} = \varphi = \pi/5$ was selected. The discretization with respect to φ involved four azimuth planes. The mesh in the peripheral stream tube involved 13 points in the tube and 24 points in the jet in the z-direction. The numerical tests led to the classical swell results $\chi = R(z_2)/r_0 = 1{\cdot}13$ for the axisymmetric Newtonian case.

5.2.2. Results for a die of square cross-section. To compute the extrudate swell surface, a peripheral stream tube limited by planes $\theta = \mathbf{g} = \varphi_0 = 0$ and $\theta = \mathbf{g} = \varphi_1 = \pi/4$ was considered owing to the symmetry properties of the duct. Several numerical tests on different meshes led us to adopt in the z-direction a similar discretization to that corresponding to the axisymmetric case. The grid in the φ-direction involved seven azimuthal planes, leading to a total of 148 unknowns according to the z-discretization. For the square duct the respective upstream and downstream cross-sections z_1 and z_2 were defined similarly to those in the circular case using the relations

$$(z_1 - z_0)/r_M = -4, \qquad (z_2 - z_0)/r_M = 10.$$

Here r_M denotes the average radius related to the square section. The half-length of the square was given by $a = 0{\cdot}781$ with $r_M = 1$.

The iterative procedure permitted direct determination of the optimal three-dimensional free surface according to the previous considerations. Figure 5(a) presents sections of the computed peripheral stream tube involving the stream surfaces $\mathscr{S}_0$ (wall and free surface), $\mathscr{S}_1$ and $\mathscr{S}_2$ for planes $z =$ constant. Figure 5(b) shows azimuthal sections of the tube $\mathscr{B}$ for planes $\varphi =$ constant, from

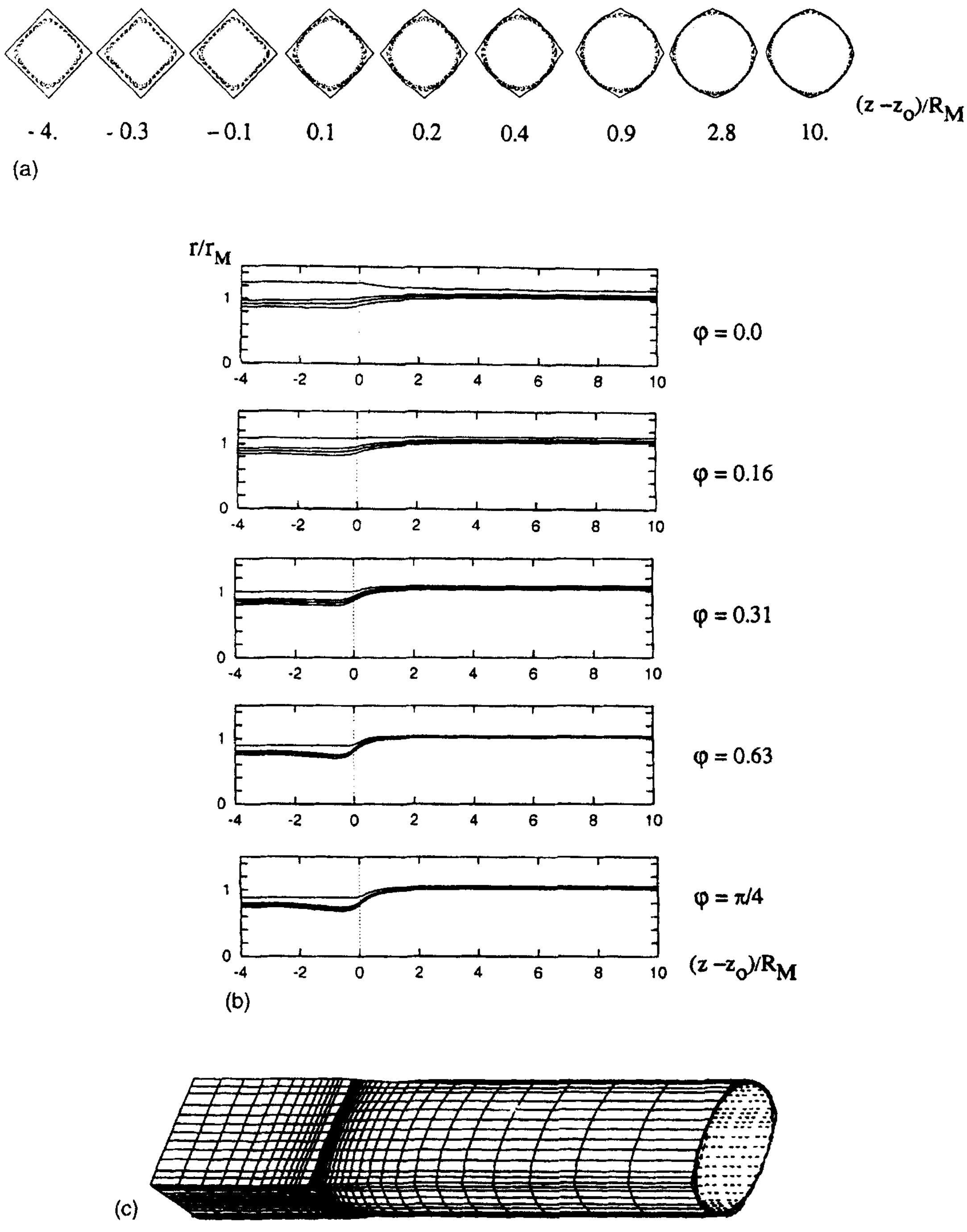

Figure 5. Computed peripheral stream tube involving stream surface $\mathfrak{S}_0$ (wall and free surface), $\mathfrak{S}_1$, $\mathfrak{S}_2$ and $\mathfrak{S}_3$ (cases (a) and (b)): (a) cross-sections of peripheral stream tube in die and jet from section z_1 to z_2; (b) azimuthal sections of tube $\mathfrak{B}$ for planes $\varphi =$ constant, from $\varphi = 0$ to $\pi/4$; (c) three-dimensional view of computed free surface, featuring discretization points

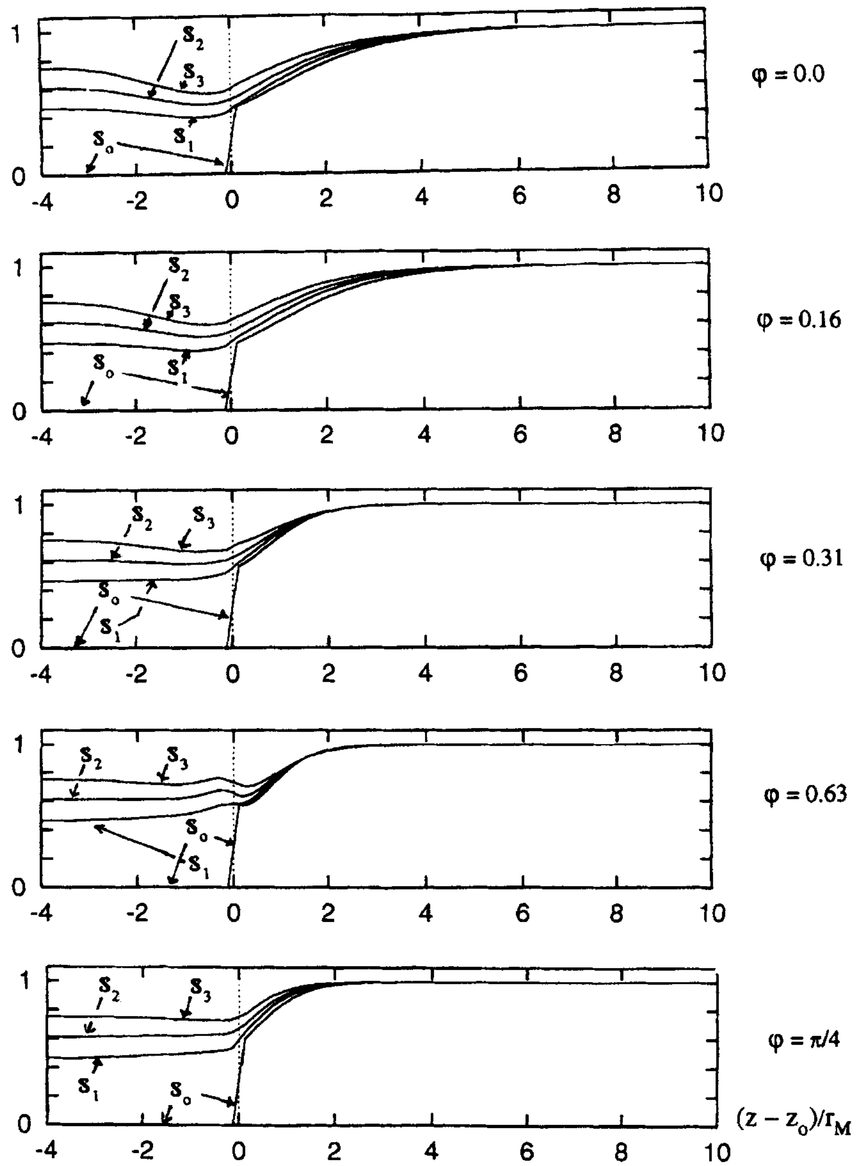

Figure 6. Dimensionless velocity component w/w_2 (w_2 is the solid flow velocity) for streamlines related to surfaces $\mathfrak{S}_0$ (wall and free surface), $\mathfrak{S}_1$, $\mathfrak{S}_2$ and $\mathfrak{S}_3$ in various azimuthal planes

$\varphi = 0$ to $\pi/4$, and the general jet shape is depicted in Figure 5(c). It may be observed that the liquid swells or retracts depending on the azimuthal angle φ. The swell ratio at $\theta = \varphi = \pi/4$ is found to be $1{\cdot}18 \pm 0{\cdot}015$, which is close to the computed swell value (1·18) given by Wambersie and Crochet.[6] The ratio corresponding to the relative reduction in size of the jet radius at $\varphi = 0$ is found to be 0·925, which is consistent with numerical results in the literature.

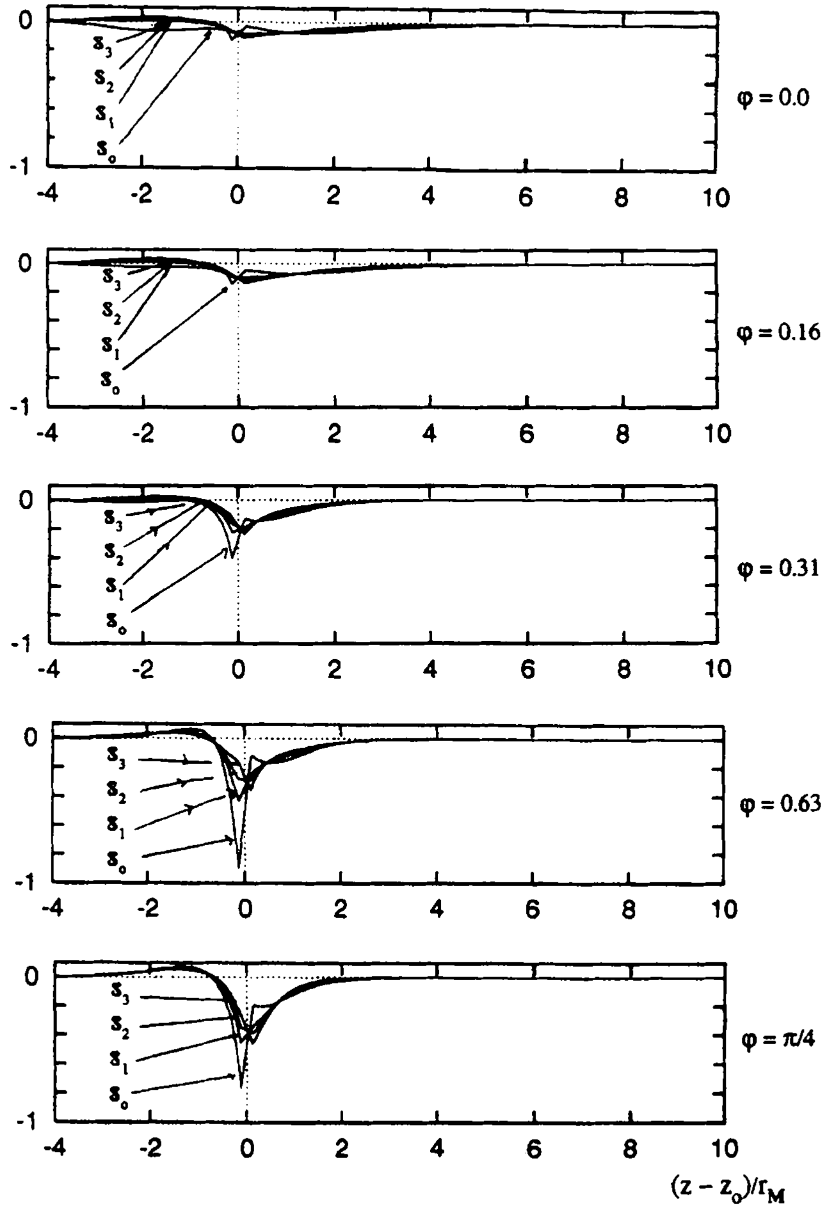

Figure 7. Dimensionless stress components $T^{zz}/T^{zz}_{w}(\varphi)$ along streamlines of surfaces $\mathfrak{S}_0$, $\mathfrak{S}_1$, $\mathfrak{S}_2$ and $\mathfrak{S}_3$ for various azumuthal sections $\theta = g \approx \varphi$, from $\theta = 0$ to $\pi/4$ (peripheral stream tube)

From basic considerations of stream tube analysis the flow streamlines are determined by the intersection of surfaces f and g. Changes in the mapping function g are to be related to the 'warping' of the streamline curves, which are plane in two-dimensional cases. The calculations revealed that the function g is practically a constant versus the variables R and Z in the peripheral stream tube. Accordingly, in this flow region the streamlines lie in the same plane as in two-dimensional flow situations.

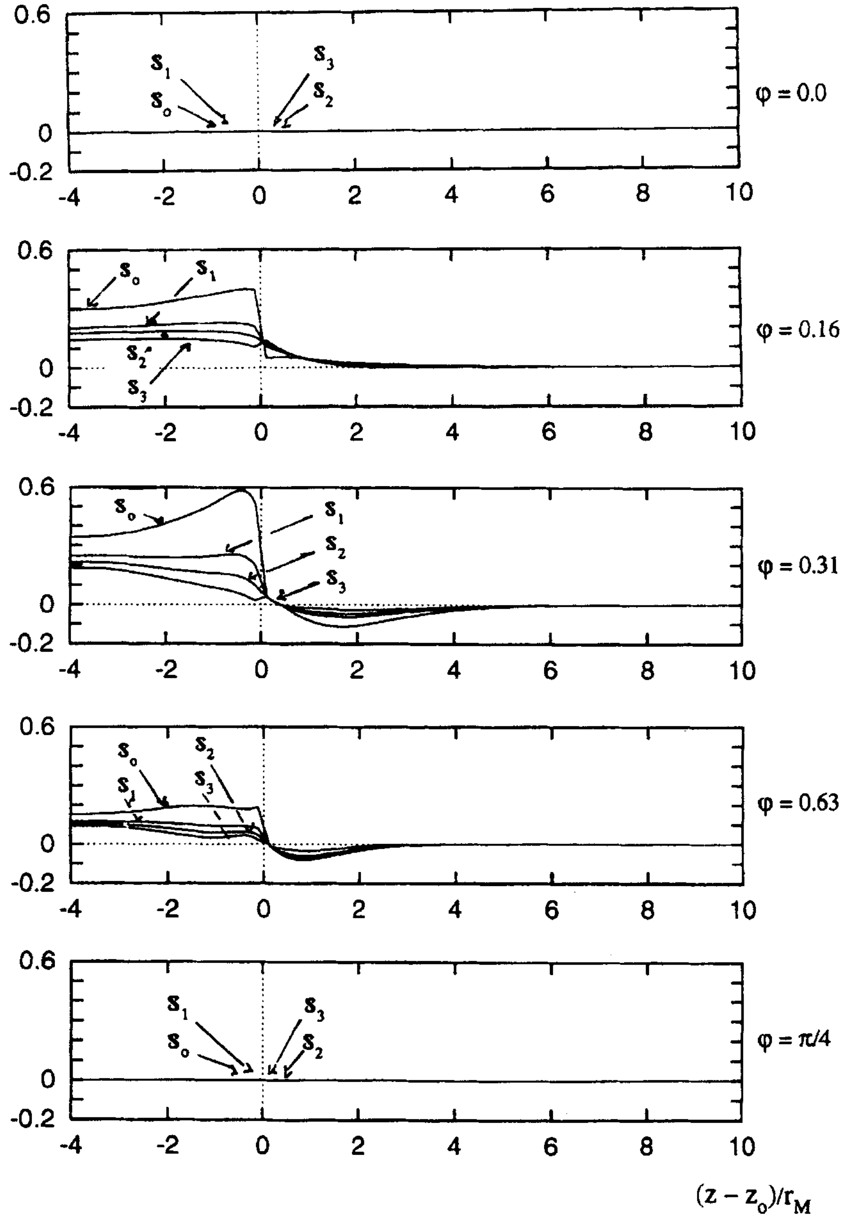

Figure 8. Dimensionless stress components $T^{\theta z}/T_{rz}(\varphi)$ along streamlines of surfaces $\mathfrak{S}_0$, $\mathfrak{S}_1$, $\mathfrak{S}_2$ and $\mathfrak{S}_3$ for various azimuthal sections $\theta = \mathrm{g}\varphi$, from *thetaq* $= 0$ to $\pi/4$ (peripheral stream tube)

Plots of the axial velocity component w related to the streamlines of surfaces $\mathscr{S}_0$ (wall and free surface), $\mathscr{S}_1$, $\mathscr{S}_2$ and $\mathscr{S}_3$ are shown in Figure 6 for various azimuthal sections. It can be observed that a constant velocity is obtained in the jet for sections close to the exit plane at $z = z_0$. The dimensionless stress components T^{zz} and $T^{\theta z}$ related t the streamlines of surfaces $\mathscr{S}_0$, $\mathscr{S}_1$ and $\mathscr{S}_2$ are shown in Figures 7 and 8 respectively for various azimuthal sections $\theta = \mathrm{g} \approx \varphi$, from $\theta = 0$ to $\pi/4$, in the computed peripheral stream tube. In these plots the wall stress components $T^{zz}_{\mathrm{w}}(\varphi)$ and $T^{rz}_{\mathrm{w}}(\varphi)$ at the upstream section z_1 are used as dimensionless factors. Singularity stress effects, which attenuate from the boundary surface $\mathscr{S}_0$ to the inside, may be observed particularly for the component T^{zz}. It should also be pointed out that the component $T^{\theta z}$, which is found to be zero in planes $\theta = g = \varphi = 0$ and $\theta = g = \varphi = \pi/4$ for reasons of symmetry (Figure 7), vanishes in two-dimensional flow situations.

6. CONCLUSIONS

In this paper a numerical method based on streamtube analysis has been developed for swell problems of a Newtonian fluid in a three dimensional flow situation. Some distinguishing features of the streamtube formulation, notably the automatic verification of the incompressibility condition, enabled the numerical calculations to be performed for a subdomain of the total flow geometry. Owing to these possibilities in three dimensions, a limited number of unknowns were considered, leading to reductions in computing time and storage area in comparison with classic flow analysis. Although the method was applied to the Newtonian case, the elements presented in this paper may be generalized to viscoelastic fluids, including memory-integral constitutive equations, as considered in previous two-dimensional studies involving stream tube analysis. As already pointed out, the use of rectilinear transformed lines of open streamlines related to the swell problem enables problems involved in evaluating kinematic tensors and stresses to be significantly reduced.[20,21] The approximation adopted for the mapping function f related to the shape of the streamlines, which results from a generalization of the Batchelor–Horsfall equation, may still be considered as realistic in 3D swell problems.

From the numerical point of view the simple mapped computational domain led to the definition of simple discretization schemes for the equations. The possibility of computing the free surface and singularity effects directly by considering an unchanged grid in the mapped peripheral stream tube, as well as the efficiency of the Levenberg–Marquardt algorithm for solving the equations, is to be underlined.

The results obtained by the present method are consistent with numerical data in the literature. This work is a first step towards computation of 3D free surface flows for fluids obeying more sophisticated constitutive equations.

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