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COMPARISON BETWEEN THE TRACTION AND PRESSURE-IMPOSED BOUNDARY CONDITIONS IN FINITE ELEMENT FLOW ANALYSIS

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SUMMARY

A formulation is developed to impose pressure-prescribed boundary conditions in the penalty finite element method. Some numerical experiments for the Poiseuille flow problem are performed to compare it with the conventional traction-prescribed boundary condition. Also the incorrectness of the traction-free outlet boundary condition for contained flows is studied with explanatory numerical examples. Discussion is focused on the inlet and outlet boundary conditions to simulate fully developed flows. Finally, the three-dimensional flow in a bifurcated pipe is analysed with the proposed formulation.

KEY WORDS Penalty Finite Element Method Navier–Stokes Equation Boundary Condition Fully Developed Flow Three-dimensional Flow

INTRODUCTION

Since pressure is a physically measurable quantity, we sometimes encounter problems where only the pressure difference between the inlet and outlet is known in fully developed flows. Our aim in this paper is to compute the fully developed flow in a three-dimensional bifurcated pipe where only pressure differences are known *a priori*. The question is what kind of boundary condition is appropriate for this problem. For two-dimensional fully developed, contained flow, the common boundary condition used in the finite element method is the imposition of a parabolic velocity profile at the inlet and a traction-free condition at the outlet. However, the flow rate of the influx is unknown in general, because the local pressure gradient at the inlet depends on the configuration of the pipe, which may contain an orifice or an obstacle in it or may be bifurcated. Furthermore, even the inlet velocity profile cannot be assumed in the three-dimensional flows, owing to the arbitrary cross-sectional shape of the pipe. Therefore, specification of the velocity profile at the inlet is impractical for our case.

As for the outlet boundary, the traction-free condition has commonly been used by most finite element practitioners, but it is incorrect since the value of traction is non-zero even for fully developed flow, and unknown in general. Instead of imposition of velocity or traction, it seems very natural to specify pressure values at inlet and outlet because pressure is constant on the plane normal to the local streamline in fully developed flows, although care should be taken so as not to violate mass conservation.[1] If one uses the mixed method[2] of velocity and pressure,

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the pressure-prescribed boundary conditions can be specified as the essential boundary condition of pressure. In the penalty finite element method,[3-9] on the other hand, it is impossible to impose pressure values as an essential boundary condition, since pressure does not appear explicitly as a variable in practical computations.

In the present paper, we propose a new formulation in which the pressure-prescribed boundary condition can be incorporated as the natural boundary condition in the penalty finite element formulation. To demonstrate the formulation, it is applied to the Poiseuille flow problem, where incorrectness of traction free outlet boundary condition is also shown numerically. Finally, the three-dimensional flow in a bifurcated pipe is analysed with the proposed formulation.

THEORY

Basic equations

The basic equations for the steady incompressible and viscous fluid flow are written as follows:

$$u_{i,i} = 0, \tag{1}$$

$$u_j u_{i,j} + \frac{1}{\rho} p_{,i} - \frac{1}{\rho} \tau_{ij,j} = 0, \tag{2}$$

where the usual Einstein summation convention is used and the subscripts i and j run from 1 to 3. The variables u_i, p, τ_{ij} and ρ imply the ith component of velocity, pressure, deviatoric stress and density, respectively.

The following equation is given formally if the constraint condition (1) is satisfied by the penalty function method:[3-9]

$$p = -\lambda u_{i,i} (\lambda \to \infty), \tag{3}$$

where λ is called the penalty parameter and a large positive number, say 10^7, is selected for it in an actual computation.

The deviatoric stress τ_{ij} for a Newtonian fluid is given as follows:

$$\tau_{ij} = \eta (u_{i,j} + u_{j,i}), \tag{4}$$

where η is the viscosity of the fluid.

Boundary conditions

The following two types of boundary conditions are considered in this study to supplement equations (1) and (2).

Type 1.

$$u_i = \hat{u}_i, \quad \text{on} \quad \Gamma_v, \tag{5}$$

$$t_i = \hat{t}_i, \quad \text{on} \quad \Gamma_t, \tag{6}$$

where ($\hat{}$) denotes the prescribed value, and the traction t_i is defined as follows:

$$t_i = -p n_i + \eta (u_{i,j} + u_{j,i}) n_j, \tag{7}$$

where n_i is the ith component of the normal unit vector on the boundary.

Type 2.

$$u_i = \hat{u}_i, \quad \text{on} \quad \Gamma_v, \tag{8}$$

$$p = \hat{p}, \quad \text{on} \quad \Gamma_p. \tag{9}$$

The velocity is imposed as the essential boundary condition, whereas, the traction and pressure are imposed as the natural boundary conditions. We assume that the essential and natural boundary conditions cover the whole boundary and do not overlap each other.

Here special care should be taken to impose the pressure value, because imposition of pressure could violate mass conservation[1] and specification of pressure alone is insufficient, since specification of three boundary conditions is required in three-dimensional problems. The pressure is, however, the most relevant variable in simulating the fully developed flows. If one considers the fully developed flow in an infinite straight pipe parallel to the z-direction, the Navier–Stokes equations and incompressibility constraint are reduced to the following equations:

$$\frac{\partial p}{\partial x} = \frac{\partial p}{\partial y} = 0, \tag{10}$$

$$v\left(\frac{\partial^2 w}{\partial x^2} + \frac{\partial^2 w}{\partial y^2}\right) = \frac{1}{\rho}\frac{\partial p}{\partial z}, \tag{11}$$

$$\frac{\partial w}{\partial z} = 0, \tag{12}$$

where w is the velocity component in the z-direction. These equations require that the pressure should be constant in any plane normal to the pipe. Therefore, the following three restrictions are imposed on the pressure-prescribed boundaries to comply with the fully developed flow conditions.

(i) The boundary surface Γ_p should be flat and normal to the longitudinal direction of the pipe.
(ii) The pressure value should be constant on the pressure-prescribed boundary on Γ_p.
(iii) The pipe should be straight and long enough to realize the fully developed flow.

Although there is ambiguity in the above restrictions, we expect that these restrictions would be sufficient to specify the pressure values consistently. At least, these restrictions are necessary conditions for fully developed flows.

Weak formulations

In this section, two types of weak formulation are given, corresponding to the two types of the boundary conditions mentioned above.

Type 1. Substituting equation (4) into equation (2), a weak form of equation (2) is derived by the weighted residual method as follows:

$$\int_\Omega \left\{ w_k u_j u_{i,j} + \frac{1}{\rho} w_k p_{,i} - v w_k (u_{i,j} + u_{j,i})_{,j} \right\} \mathrm{d}\Omega = 0, \tag{13}$$

where Ω denotes the whole domain and w_k is a weighting function which is assumed to be zero on the velocity-prescribed boundary Γ_v. Applying the Green–Gauss theorem to the second and the third terms of equation (13), we obtain the following equations:

$$\int_{\Omega}\left\{w_k u_j u_{i,j}-\frac{1}{\rho}w_{k,i}p+\nu w_{k,j}(u_{i,j}+u_{j,i})\right\}\mathrm{d}\Omega$$
$$=-\frac{1}{\rho}\int_{\Gamma}w_k p n_i\,\mathrm{d}\Gamma+\nu\int_{\Gamma}w_k(u_{i,j}+u_{j,i})n_j\,\mathrm{d}\Gamma. \tag{14}$$

Substitution of equation (6) into the right-hand side integral of equation (14) leads to the following equation:

$$\int_{\Omega}\left\{w_k u_j u_{i,j}-\frac{1}{\rho}w_{k,i}p+\nu w_{k,j}(u_{i,j}+u_{j,i})\right\}\mathrm{d}\Omega=\frac{1}{\rho}\int_{\Omega_t}w_k\hat{t}_i\,\mathrm{d}\Gamma. \tag{15}$$

Here we employed the condition: $w_k=0$ on Γ_v. Equation (15) implies that the traction t_i can be introduced as a natural boundary condition.

Type 2. In order to introduce the pressure-prescribed boundary condition into equation (14), the deviatoric stress term in the right-hand side of equation (14) is transferred to the left-hand side of the equation as follows:

$$\int_{\Omega}\left\{w_k u_j u_{i,j}-\frac{1}{\rho}w_{k,i}p+\nu w_{k,j}(u_{i,j}+u_{j,i})\right\}\mathrm{d}\Omega-\nu\int_{\Gamma_p}w_k(u_{i,j}+u_{j,i})n_j\,\mathrm{d}\Gamma$$
$$=-\frac{1}{\rho}\int_{\Gamma_p}w_k\hat{p}n_i\,\mathrm{d}\Gamma, \tag{16}$$

where the condition: $w_k=0$ on Γ_v is employed. Equation (16) shows that one may prescribe the pressure value on the boundary Γ_p as a natural boundary condition.

It should be noted that equation (16) contains both volume and surface integrals on the left-hand side, whereas the conventional formulation (15) contains only a volume integral. Although we are unprepared to state the mathematical property regarding formulation (16), we suppose that the solution exists under physically reasonable conditions. Our belief rests on the fact that a similar formulation has often been used in heat conduction analyses with radiation or heat transfer boundary conditions. The weak form of the steady heat conduction equation is written as follows:

$$\kappa\int_{\Omega}T^*_{,i}T_{,i}\,\mathrm{d}\Omega=-\int_{\Gamma}T^*q\,\mathrm{d}\Gamma, \tag{17}$$

where κ is the heat conductivity and T, T^* and q stand for temperature, weighting function and heat flux, respectively. If the boundary Γ is the heat transfer boundary, the heat flux q is replaced by the following relation:

$$q=h(T-T_\infty), \tag{18}$$

where h is the heat transfer coefficient and T_∞ the bulk temperature. Then, one must solve the following equation with an unknown natural boundary condition of heat flux:

$$\kappa\int_{\Omega}T^*_{,i}T_{,i}\,\mathrm{d}\Omega+h\int_{\Gamma}T^*T\,\mathrm{d}\Gamma=h\int_{\Gamma}T^*T_\infty\,\mathrm{d}\Gamma. \tag{19}$$

Although the existence of the solution is still an open question to our knowledge, this formulation is used in many engineering applications.

In the following, we consider the extension of equation (16) to another type of formulation which is derived in the same way. As mentioned in the Introduction, the traction values are non-zero at the outlet even for fully developed flows, and are unknown in general. Taylor *et al.*[10] have proposed an iterative procedure for the evaluation and imposition of non-zero tractions on boundaries where advection is appreciable. The iterative solutions for v_i and p, if converged, would satisfy the following equation:

$$\int_{\Omega}\left\{w_k u_j u_{i,j} - \frac{1}{\rho} w_{k,i} p + \nu w_{k,j}(u_{i,j} + u_{j,i})\right\} \mathrm{d}\Omega$$

$$+ \frac{1}{\rho}\int_{\Gamma_t} w_k p n_i \,\mathrm{d}\Gamma - \nu \int_{\Gamma_t} w_k (u_{i,j} + u_{j,i}) n_j \,\mathrm{d}\Gamma = 0, \tag{20}$$

where u_i and p in both volume and surface integrals are considered as unknowns. Taylor *et al.*[10] have obtained successful results and explained the physical meaning of such a boundary condition by the statement that 'no disturbances are propagated in an upstream direction from the downstream boundary'. Therefore, we expect that the formulation (20) would be applicable to the problems of advection-dominant flows and buoyancy-influenced flows,[11] although the formulation (20) is not the main subject of this paper.

Finite element formulations

The velocity u_i and the weighting function w_k are discretized in the usual finite element manner as follows:

$$u_i = u_{\alpha i}\Phi_\alpha, \tag{21}$$

$$w_k = w_{\alpha k}\Phi_\alpha \tag{22}$$

where Φ_α is the trilinear interpolation function with respect to node α, and $u_{\alpha i}$ and $w_{\alpha k}$ stand for the values of u_i and w_k at node α, respectively. The pressure p and weighting function p^* for equation (3) are approximated by the piecewise constant function Ψ_α as follows:

$$p = p_\alpha \Psi_\alpha, \tag{23}$$

$$p^* = p^*_\alpha \Psi_\alpha. \tag{24}$$

Since the discretized pressures can be eliminated from equations (15) and (16), the following matrix equations are obtained finally.

Type 1.

$$B_{\alpha\beta\gamma j} u_{\beta j} u_{\gamma i} + C_{\alpha\beta ij} u_{\beta j} + D_{\alpha\beta ij} u_{\beta j} = T_{\alpha i}. \tag{25}$$

Type 2.

$$B_{\alpha\beta\gamma j} u_{\beta j} u_{\gamma i} + C_{\alpha\beta ij} u_{\beta j} + D_{\alpha\beta ij} u_{\beta j} + S_{\alpha\beta ij} u_{\beta j} = P_{\alpha i}, \tag{26}$$

where

$$B_{\alpha\beta\gamma j} = \int_{\Omega} \Phi_\alpha \Phi_\beta \Phi_{\gamma,j} \,\mathrm{d}\Omega, \tag{27}$$

$$C_{\alpha\beta ij} = \frac{\lambda}{\rho}\int_{\Omega} \Phi_{\alpha,i} \,\mathrm{d}\Omega \int_{\Omega} \Phi_{\beta,j} \,\mathrm{d}\Omega \Big/ \int_{\Omega} \mathrm{d}\Omega, \tag{28}$$

$$D_{\alpha\beta ij}=\nu\int_{\Omega}(\Phi_{\alpha,j}\Phi_{\beta,i}+\Phi_{\alpha,l}\Phi_{\beta,l}\delta_{ij})\,\mathrm{d}\Omega, \tag{29}$$

$$S_{\alpha\beta ij}=-\nu\int_{\Gamma_p}(\Phi_{\alpha}\Phi_{\beta,i}n_j+\Phi_{\alpha}\Phi_{\beta l}n_l\delta_{ij})\,\mathrm{d}\Gamma, \tag{30}$$

$$T_{\alpha i}=\frac{1}{\rho}\int_{\Gamma_t}\Phi_{\alpha}\hat{t}_i\,\mathrm{d}\Gamma, \tag{31}$$

$$P_{\alpha i}=-\frac{1}{\rho}\int_{\Gamma_p}\Phi_{\alpha}\hat{p}n_i\,\mathrm{d}\Gamma. \tag{32}$$

It should be noted that equation (26) contains the matrix of surface integrals which results from the deviatoric stress on the boundary Γ_p. The velocities $u_{\alpha i}$ are obtained by the Newton–Raphson procedure, since the equations are non-linear with respect to $u_{\alpha i}$, which is due to the convective term of the Navier–Stokes equation. The algebraic equations linearized in the Newton–Raphson procedure are solved by means of the wave front method[12] to save the primary memory of the computer.

NUMERICAL RESULTS

Poiseuille flows

In order to compare the type 1 and 2 formulations, a simple fully developed flow, that is the Poiseuille flow problem, is considered in this section. Here, the discussion and computation are restricted to the two-dimensional spatial domain, although the computations are executed by the three-dimensional code. As is well known, the exact velocity components of the Poiseuille flow are given as follows:

$$u_1=-\frac{1}{2\eta}\frac{\mathrm{d}p}{\mathrm{d}x}(2by-y^2), \tag{33}$$

$$u_2=0, \tag{34}$$

where b denotes the half-width between two parallel walls and $-\mathrm{d}p/\mathrm{d}x$ the constant pressure gradient. Assuming that the pressure is unity at the inlet and zero at the outlet, the exact values of the tractions $t_i(i=1,2)$ at the inlet and outlet are calculated as follows, using the definition of the traction (7) and the exact solutions (33) and (34):

$$t_1=1,\quad t_2=\frac{\mathrm{d}p}{\mathrm{d}x}(b-y),\quad \text{at the inlet,} \tag{35}$$

$$t_1=0,\quad t_2=-\frac{\mathrm{d}p}{\mathrm{d}x}(b-y),\quad \text{at the outlet.} \tag{36}$$

Here, as shown from equation (36), it is worthy of note that the exact value of the traction is not zero at the outlet, although many analysts are using a traction-free outlet boundary condition. From equation (35) or (36), one could see that the tractions t_2 approach zero if the pressure gradient $-\mathrm{d}p/\mathrm{d}x$ approaches zero. However, according to equation (33), the velocity remains unchanged if the viscosity η is as small as the pressure gradient. Therefore, the traction-free outlet boundary condition appears to be correct only for large Reynolds number problems of

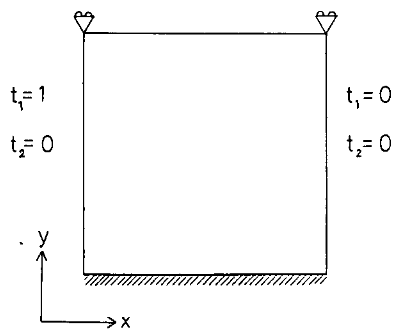

Figure 1. Inconsistent traction boundary conditions (type 1 formulation)

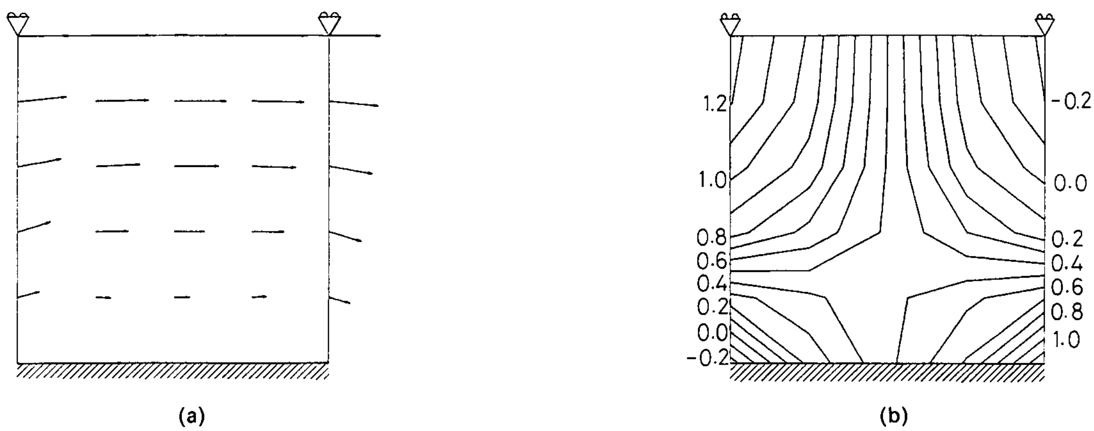

Figure 2. Numerical solutions of inconsistent traction boundary conditions (type 1 formulation): (a) velocity distribution; (b) pressure distribution

small viscous effect. This phenomenon is discussed by Leone and Gresho.[13] To study the effect of the traction-free outlet boundary condition, the flow is analysed here using the boundary conditions as shown in Figure 1. The traction t_2 at both inlet and outlet is assumed to be zero. The computational domain is divided into $4 \times 5 \times 1$ brick elements in the x-, y- and z-directions, respectively. The material and geometrical constants are given as follows:

$$\eta = 1, \quad b = L = 1, \tag{37}$$

where L is the length between the inlet and the outlet. If one takes maximum velocity in the domain as the representative velocity and $2b$ as the representative length, the Reynolds number is estimated to be unity for the analytical solution of the Poiseuille flow. Figures 2(a) and 2(b) show, respectively, the velocity and pressure distributions. Both are far from the analytical solution, as expected. The easiest way to remedy the solution is to impose the zero cross-stream velocity, that is $u_2 = 0$ at the inlet and outlet. However, it needs more complicated programming to impose such a condition, particularly on inclined boundaries, and this boundary condition may cause numerical oscillations in some cases,[14] whereas the type 1 formulation is still useful if the consistent tractions according to the equations (35) and (36) are used.

Next, we apply the type 2 formulation to the Poiseuille flow problem. The boundary conditions are depicted in Figure 3. The material and geometrical constants and mesh subdivisions are the

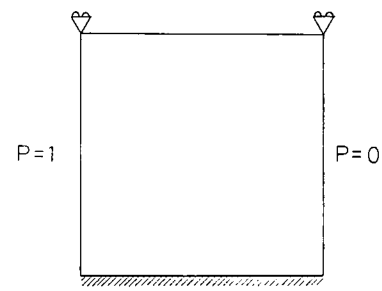

Figure 3. Boundary conditions for the Poiseuille flow problem (type 2 formulation)

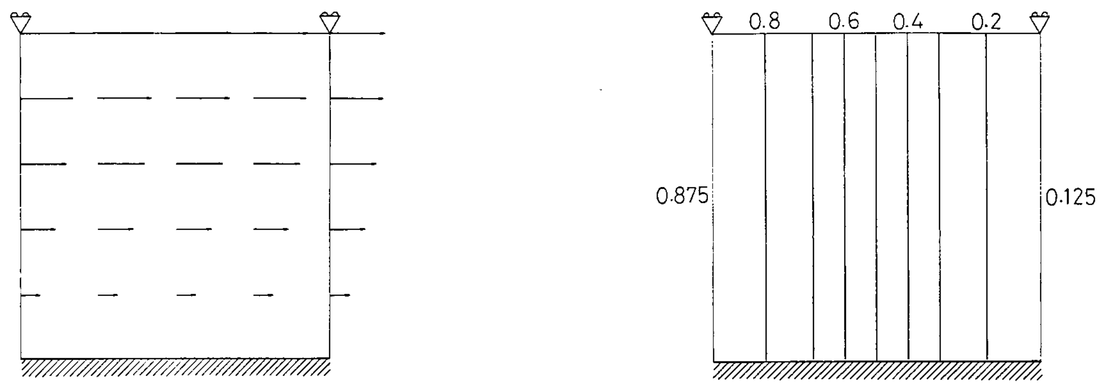

Figure 4. Numerical solutions of the Poiseuille flow (type 2 formulation): (a) velocity distribution; (b) pressure distribution

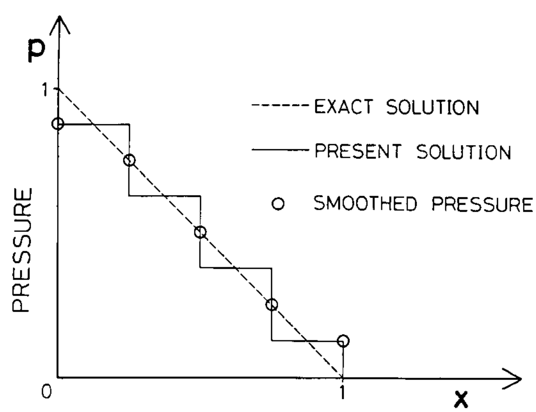

Figure 5. Comparison of analytical and numerical solutions for pressure

same as the former ones. Figures 4(a) and 4(b) show velocity and pressure distributions, respectively, both of which exactly agree with the analytical solution. The reason why the intervals between two neighbouring pressure contour lines are unequal in Figure 4(b) is the smoothing procedure through which the pressure value obtained by equation (3) for each element is redistributed to each node for plotting purposes using the least-squares method. The original pressure before the smoothing procedure is given in comparison with the exact solution and the smoothed pressure in Figure 5, which shows the good agreement between the original pressure and the exact one.

From the above numerical experiments, it turns out that the type 2 formulation is quite straightforward to specify the inlet and outlet boundary conditions, whereas the type 1 formulation needs to evaluate a non-zero traction value *a priori* which is impractical in general, especially for three-dimensional problems.

Three-dimensional flow in a bifurcated pipe

A bifurcated pipe is one of the most important components in chemical, nuclear and other plants. Here, the flow around the junction of the bifurcated pipe is analysed, as shown in Figure 6. In this problem, the flow is driven by the pressure differences between the inlets and the outlet and is assumed fully developed near the inlets and outlet. It is hardly possible to calculate the analytical velocity distributions at the inlets or outlet because the flow rates through the inlets or outlet are unknown owing to the bifurcation of the pipe even though the velocity profiles can be determined for such simple cross-sections. Therefore, the traction values at the inlets and outlet cannot be estimated *a priori.* The alternative way to impose the traction values is the use of the iterative procedure proposed by Taylor *et al.*[10] Such an iteration method, however, requires additional computational efforts, even if it is very effective for advection-dominant problems.

On the other hand, the application of pressure-prescribed boundary conditions to this problem is very straightforward. Here, the boundary conditions are imposed as follows:

$$\begin{aligned} u_1 = u_2 = u_3 &= 0, && \text{on the pipe wall,} \\ u_2 &= 0, && \text{on the symmetry plane,} \\ p &= 1, && \text{at inlets A and B,} \\ p &= 0, && \text{at the outlet.} \end{aligned} \tag{38}$$

The finite element mesh subdivisions consist of 648 elements and 996 nodal points for the half portion of the flow because of the symmetry condition (see Figure 7). The material constants, such as viscosity and density of the fluid are assumed to be unity in this case. The computed velocity and pressure on the symmetry plane are shown in Figures 8(a) and (b), respectively. These results seem to be reasonable and indicate the validity of the Type 2 formulation.

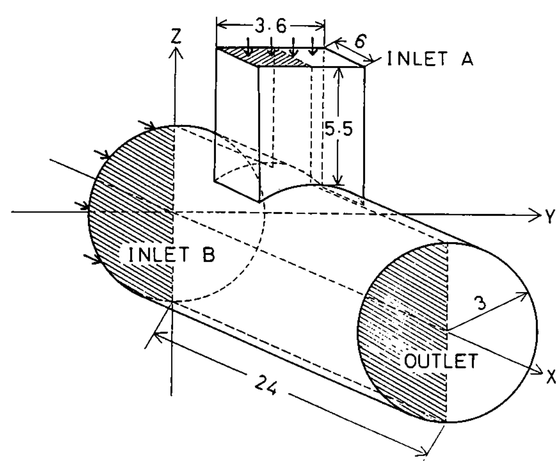

Figure 6. Problem description of the flow in a bifurcated pipe

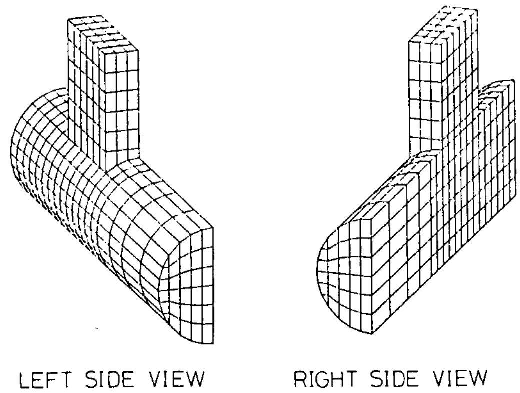

Figure 7. Finite element subdivisions of the bifurcated pipe

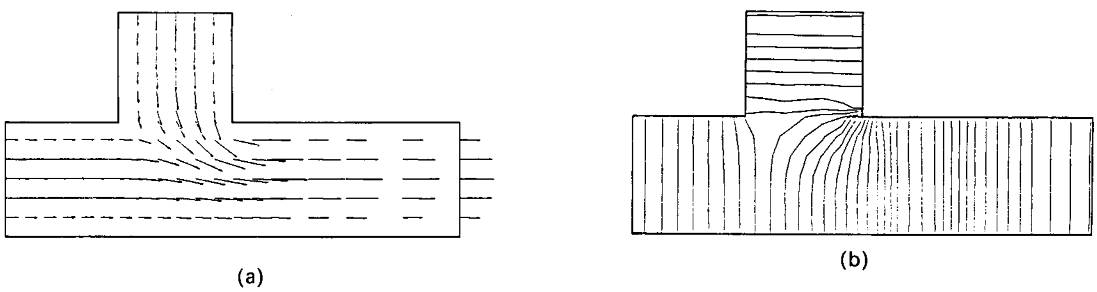

Figure 8. Numerical solutions on the symmetry plane (type 2 formulation): (a) velocity distribution; (b) pressure distribution

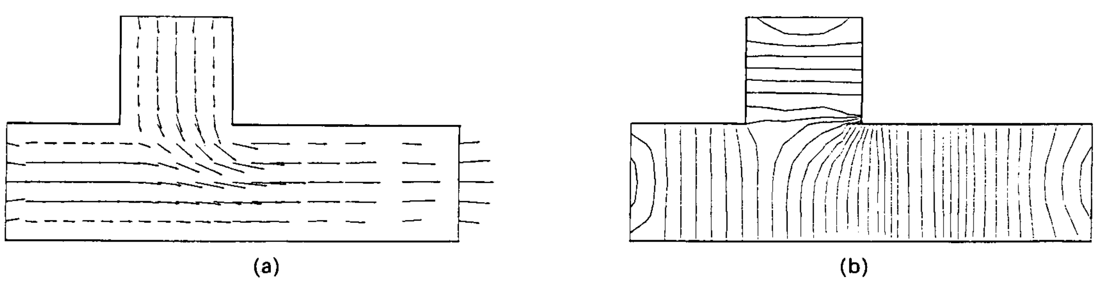

Figure 9. Numerical solutions by traction-free outlet and analogous inlet boundary conditions (type 1 formulation): (a) velocity distribution; (b) pressure distribution

We also demonstrate the incorrectness of the traction free outlet boundary condition, using the Type 1 formulation with the following boundary conditions:

$$
\begin{aligned}
&u_1 = u_2 = u_3 = 0, \quad \text{on the pipe wall,} \\
&u_2 = 0, \quad t_1 = t_3 = 0, \quad \text{on the symmetry plane,} \\
&t_1 = t_2 = 0, \quad t_3 = -1, \quad \text{at inlet A,} \\
&t_1 = 1, \quad t_2 = t_3 = 0, \quad \text{at inlet B,} \\
&t_1 = t_2 = t_3 = 0, \quad \text{at the outlet,}
\end{aligned} \tag{39}
$$

where the inlet traction values are given by analogy with the outlet traction values. The computational results for velocity and pressure are shown in Figures 9(a) and 9(b), respectively. Figure 9(a) shows converging velocity profiles at the inlets and a diverging one at the outlet, accompanied by the distorted pressure contours of Figure 9(b). These solutions indicate that the traction-free outlet boundary condition and an analogous inlet boundary condition seem to be practically incorrect, even though such boundary conditions are prevalent in the finite element flow analyses.

CONCLUSION

Our numerical results have demonstrated that the traction-free outlet boundary condition which many finite element practitioners are using is incorrect even for fully developed flows. In our formulation, on the other hand, the surface integral of the deviatoric stress, which causes non-zero traction values at the boundaries, is treated as unknown and is solved together with the volume integrals. This formulation makes it easy to specify boundary conditions for fully developed flows by imposing pressure values. The numerical results of the two-dimensional Poiseuille flow and the three-dimensional flow in a bifurcated pipe support the validity of the proposed formulation.

The application of the Type 2 formulation is limited to the fully developed flows in this study. However, we have also suggested another type of formulation which is derived in the same manner as the Type 2 formulation. Although the numerical verifications have not been performed yet, we expect that the formulation (20) would be effective for advection-appreciable flows as well as buoyancy-influenced flows.

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