A Compatibility Error in the Formulation of a Popular General Purpose Finite Difference Scheme for the Solution of Elliptic Partial Differential Equations

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In this paper, the finite difference formulation used in a popular generalized procedure (1) for the solution of turbulent flow heat and mass transfer problems is shown to contain a compatibility error when the scheme is applied to certain geometries. Following a brief description of the procedure in question, a corrected form of the finite difference equations is proposed. A heat conduction problem and a laminar flow problem, for which theoretical solutions exist, are used to substantiate the modifications.

INTRODUCTION

Complex problems in fluid mechanics and heat and mass transfer are frequently solved nowadays by numerical methods. In the numerical solution of the coupled set of partial differential equations pertinent to these problems, a popular approach is that using finite difference schemes. Each new problem may be programmed separately but a generalization of programmes to solve various classes of problems is clearly of much value. In this connection the work of Gosman *et al.* (**1**) warrants special mention. This now familiar procedure of solving elliptic equations which describe a wide range of real problems has been used extensively by other workers in this field (**2**), (**3**). The procedure is designed to cater for any two-dimensional axisymmetric geometry. Wilson (**2**) and Launder *et al.* (**3**), for example, have employed the method successfully for the case of fully developed turbulent flow in straight rectangular ducts. In their study of a new turbulence model (**4**), the present authors have also adopted the method proposed by Gosman *et al.* (**1**) and found the procedure entirely satisfactory for the rectangular duct geometries considered. However, extension of the use of the method to two-dimensional geometries in which the metric coefficients are functions of the co-ordinates has not met the simple criterion of convergence to a known exact solution as the mesh size is decreased. For example, using the method to compute the fully developed laminar velocity profile in a circular pipe (using polar co-ordinates) will always give a result for the centreline velocity which is twice the known exact value. This will be the case no matter what mesh size is used. It is shown later that in such cases the Gosman *et al.* formulation is incompatible with the original governing differential equations, essentially due to the neglect of a first-order derivative in the finite difference equations.

It is therefore necessary to briefly retrace some of the Gosman *et al.* analysis and for this purpose the notation which has previously been adopted will be used here. A modification will then be proposed in order to accommodate the influence of the co-ordinate system completely and finally the corrected finite difference equations will be tested using some simple examples.

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THE GOSMAN *et al.* PROCEDURE

Using the generalized orthogonal co-ordinate system for two-dimensional axisymmetric flow shown in Fig. 1, Gosman *et al.* (**1**), derive the following 'compact' partial differential equation which embodies the conservation laws of mass, momentum, and energy as well as the transport equations for turbulence quantities:

$$a_\phi \left\{\frac{\partial}{\partial \xi_1}\left(\phi \frac{\partial \psi}{\partial \xi_2}\right) - \frac{\partial}{\partial \xi_2}\left(\phi \frac{\partial \psi}{\partial \xi_1}\right)\right\} - \left\{\frac{\partial}{\partial \xi_1}\left(b_\phi \frac{l_2}{l_1} r \frac{\partial}{\partial \xi_1}(c_\phi \phi)\right)\right\} - \frac{\partial}{\partial \xi_2}\left\{b_\phi \frac{l_1}{l_2} r \frac{\partial}{\partial \xi_2}(c_\phi \phi)\right\} + l_1 l_2 r d_\phi = 0 \qquad (1)$$

where l_1 and l_2 are the metric coefficients for the ξ_1 and ξ_2 co-ordinate directions defined by

$$l_1 = \frac{dS_1}{d\xi_1}, \qquad l_2 = \frac{dS_2}{d\xi_2}. \qquad (2)$$

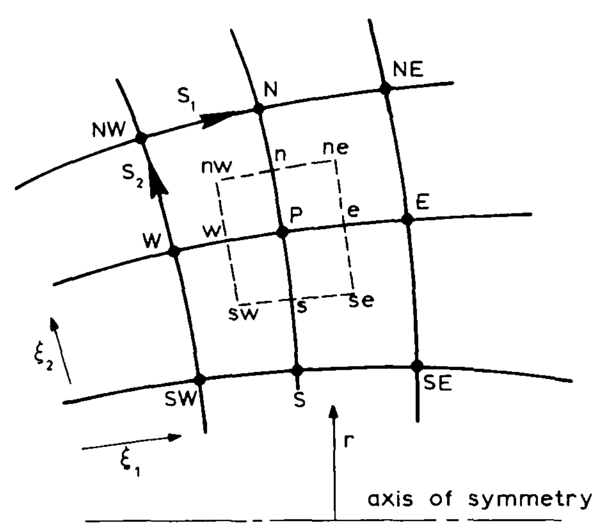

Fig. 1. Finite difference grid for the Gosman *et al.* (**1**) formulation

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S_1 and S_2 are the distance co-ordinates along the lines of constant ξ_2 and ξ_1 respectively, ϕ is any dependent variable which is a function of the co-ordinates ξ_1 and ξ_2, ψ is the stream function, and the coefficients a_ϕ, b_ϕ, c_ϕ and the source term d_ϕ depend on the physical significance of ϕ and the particular co-ordinate system.

Equation (1) is integrated over the dotted area shown in Fig. 1 giving

$$\int_{\xi_{2s}}^{\xi_{2n}}\int_{\xi_{1w}}^{\xi_{1e}} a_\phi \left\{\frac{\partial}{\partial\xi_1}\left(\phi\frac{\partial\psi}{\partial\xi_2}\right) - \frac{\partial}{\partial\xi_2}\left(\phi\frac{\partial\psi}{\partial\xi_1}\right)\right\} d\xi_1\, d\xi_2$$
$$-\int_{\xi_{2s}}^{\xi_{2n}}\int_{\xi_{1w}}^{\xi_{1e}} \left\{\frac{\partial}{\partial\xi_1}\left(b_\phi\frac{l_2}{l_1}r\frac{\partial(c_\phi\phi)}{\partial\xi_1}\right)\right.$$
$$\left.+\frac{\partial}{\partial\xi_2}\left(b_\phi\frac{l_1}{l_2}r\frac{\partial(c_\phi\phi)}{\partial\xi_2}\right)\right\} d\xi_1\, d\xi_2$$
$$+\int_{\xi_{2s}}^{\xi_{2n}}\int_{\xi_{1w}}^{\xi_{1e}} l_1 l_2 r d_\phi\, d\xi_1\, d\xi_2 = 0$$

The first and third integrals are dealt with correctly by Gosman *et al.* The compatibility error occurs in representing the second integral in finite difference terms. Hence this integral will now be considered in detail.

Integrating once gives

$$\int_{\xi_{2s}}^{\xi_{2n}}\int_{\xi_{1w}}^{\xi_{1e}} \left\{\frac{\partial}{\partial\xi_1}\left(b_\phi\frac{l_2}{l_1}r\frac{\partial(c_\phi\phi)}{\partial\xi_1}\right)\right.$$
$$\left.+\frac{\partial}{\partial\xi_2}\left(b_\phi\frac{l_1}{l_2}r\frac{\partial}{\partial\xi_2}(c_\phi\phi)\right)\right\} d\xi_1\, d\xi_2$$
$$=\int_{\xi_{2s}}^{\xi_{2n}}\left\{\left(\frac{b_\phi l_2 r}{l_1}\right)_e\left(\frac{\partial}{\partial\xi_1}(c_\phi\phi)\right)_e\right.$$
$$\left.-\left(\frac{b_\phi l_2 r}{l_1}\right)_w\left(\frac{\partial}{\partial\xi_1}(c_\phi\phi)\right)_w\right\} d\xi_2$$
$$+\int_{\xi_{1w}}^{\xi_{1e}}\left\{\left(\frac{b_\phi l_1 r}{l_2}\right)_n\left(\frac{\partial}{\partial\xi_2}(c_\phi\phi)\right)_n\right.$$
$$\left.-\left(\frac{b_\phi l_1 r}{l_2}\right)_s\left(\frac{\partial}{\partial\xi_2}(c_\phi\phi)\right)_s\right\} d\xi_1$$

Because of the similarity of the terms it is sufficient to consider only one. Gosman *et al.* consider the term

$$I_d = \int_{\xi_{2s}}^{\xi_{2n}}\left(\frac{b_\phi l_2 r}{l_1}\right)_e\left(\frac{\partial}{\partial\xi_1}(c_\phi\phi)\right)_e d\xi_2$$

and using eqs. (2) derive

$$I_d = \int_{S_{2s}}^{S_{2n}} (b_\phi r)_e\left(\frac{\partial}{\partial S_1}(c_\phi\phi)\right)_e dS_2$$

which is clearly incorrect since lines of constant ξ_1 or ξ_2 are *not* lines of constant S_1 or S_2 if the metric coefficients l_1 or l_2 are functions of the co-ordinates.

The correct derivation is

$$I_d = \int_{S_{2se}}^{S_{2ne}} (b_\phi r)_e\left(\frac{\partial}{\partial S_1}(c_\phi\phi)\right)_e dS_2$$

Hence whereas Gosman *et al.* produce the finite difference approximation

$$I_d \cong \frac{(b_{\phi E}+b_{\phi P})}{2}\frac{(r_E+r_P)}{2}\frac{(c_{\phi E}\phi_E - c_{\phi P}\phi_P)}{(S_{1E}-S_{1P})}\frac{(S_{2N}-S_{2S})}{2}$$

the correct form is

$$I_d \cong \frac{(b_{\phi E}+b_{\phi P})}{2}\frac{(r_E+r_P)}{2}\frac{(c_{\phi E}\phi_E - c_{\phi P}\phi_P)}{(S_{1E}-S_{1P})}\times\frac{1}{2}\left(\frac{(S_{2NE}-S_{2SE})}{2}+\frac{(S_{2N}-S_{2S})}{2}\right)$$

Note that the difference in the two approximations is not just a question of accuracy but one of the fundamental representations of the original partial differential equation. This point will be illustrated in the examples presented later. To conclude this section the detailed changes needed to the Gosman *et al.* formulation involve the following correcting values of B_E, B_W, B_N and B_S given on page 110 of the book (**1**):

$$B_E = \frac{(b_{\phi E}+b_{\phi P})}{16}(r_E+r_P)\left(\frac{S_{2N}-S_{2S}+S_{2NE}-S_{2SE}}{S_{1E}-S_{1P}}\right)$$
$$B_W = \frac{(b_{\phi W}+b_{\phi P})}{16}(r_W+r_P)\left(\frac{S_{2N}-S_{2S}+S_{2NW}-S_{2SW}}{S_{1P}-S_{1W}}\right)$$
$$B_N = \frac{(b_{\phi N}+b_{\phi P})}{16}(r_N+r_P)\left(\frac{S_{1E}-S_{1W}+S_{1NE}-S_{1NW}}{S_{2N}-S_{2P}}\right)$$
$$B_S = \frac{(b_{\phi S}+b_{\phi P})}{16}(r_S+r_P)\left(\frac{S_{1E}-S_{1W}+S_{1SE}-S_{1SW}}{S_{2P}-S_{2S}}\right) \quad (3)$$

EXAMPLES

Two examples have been chosen to illustrate the incompatibility of the original formulation with respect to the governing differential equation for geometries in which l_1 and l_2 are functions of the co-ordinates. The first example is extremely simple but highlights the neglect of a first-order derivative in the unmodified procedure. The second example is more involved but shows the corrective effect of the present modifications for a two-dimensional problem.

(a) Fully Developed Laminar Flow in a Circular Pipe

The momentum equation governing this simple flow is

$$\frac{\partial}{\partial r}\left(r\frac{\partial u}{\partial r}\right) - \frac{r}{\mu}\frac{\partial p}{\partial z} = 0 \quad (4)$$

with $u = 0$ on $r = a$. Here u is the flow velocity, p the pressure and μ the fluid viscosity. r is a radial co-ordinate measured from the pipe centreline and z a co-ordinate along the pipe. The pipe is of radius a. The exact solution of eq. (4) with the given boundary conditions is

$$u = \frac{1}{4\mu}\frac{\partial p}{\partial z}(r^2 - a^2) \quad (5)$$

It is instructive here to retrace again the original Gosman *et al.* finite difference formulation because then the points made in the last section appear crystal clear. Integrating eq. (4) over the dotted area of Fig. 1 (taking $\xi_2 = r$, $\xi_1 = \theta$) gives

$$\int_w^e \int_s^n \frac{\partial}{\partial r}\left(r \frac{\partial u}{\partial r}\right) dr\, d\theta - \int_w^e \int_s^n \frac{r}{\mu} \frac{\partial p}{\partial z}\, dr\, d\theta = 0$$

whence

$$\int_w^e \left\{\left(r \frac{\partial u}{\partial r}\right)_n - \left(r \frac{\partial u}{\partial r}\right)_s\right\} d\theta - \int_w^e \int_s^n \frac{r}{\mu} \frac{\partial p}{\partial z}\, dr\, d\theta = 0$$

Using relations (2) the Gosman *et al.* formulation then produces

$$\int_{S_{1w}}^{S_{1e}} \left\{\left(\frac{\partial u}{\partial S_2}\right)_n - \left(\frac{\partial u}{\partial S_2}\right)_s\right\} dS_1 - \int_{S_{1w}}^{S_{1e}} \int_{S_{2s}}^{S_{2n}} \frac{1}{\mu} \frac{\partial p}{\partial z}\, dS_2\, dS_1 = 0$$

and finally,

$$\left[\frac{u_N - u_P}{S_{2N} - S_{2P}} - \frac{u_P - u_S}{S_{2P} - S_{2S}}\right](S_{1E} - S_{1W}) - \frac{1}{2\mu} \frac{\partial p}{\partial z}(S_{1E} - S_{1W})(S_{2N} - S_{2S}) = 0$$

If (for simplicity only) a uniform mesh is assumed taken then

$$S_{2N} - S_{2P} = S_{2P} - S_{2S} = \tfrac{1}{2}(S_{2N} - S_{2S}) = \Delta r$$

and the above finite difference equation reduces to

$$\frac{u_N - 2u_P + u_S}{\Delta r^2} - \frac{1}{\mu} \frac{\partial p}{\partial z} = 0$$

which is easily recognized as a conventional finite difference approximation to the equation

$$\frac{\partial^2 u}{\partial r^2} - \frac{1}{\mu} \frac{\partial p}{\partial z} = 0$$

which with the same boundary conditions as eq. (4) has the solution

$$u = \frac{1}{2\mu} \frac{\partial p}{\partial z}(r^2 - a^2)$$

Hence the Gosman *et al.* formulation will predict a centreline velocity which is twice the exact value. It is easy to show that the modifications proposed in the earlier section give the following finite difference representation of eq. (4), namely,

$$\left[\frac{u_N + u_P}{\Delta r}\right]\left[\frac{r_N + r_P}{2}\right] - \left[\frac{u_P - u_S}{\Delta r}\right]\left[\frac{r_S + r_P}{2}\right] - \frac{1}{\mu} \frac{\partial p}{\partial z} r_P \Delta r = 0$$

which with a little manipulation gives

$$\frac{(u_N - 2u_P + u_S)}{\Delta r^2} + \frac{1}{r_P} \frac{(u_N - u_S)}{2\Delta r} - \frac{1}{\mu} \frac{\partial p}{\partial z} = 0$$

This expression agrees with a conventional finite difference approximation to eq. (4).

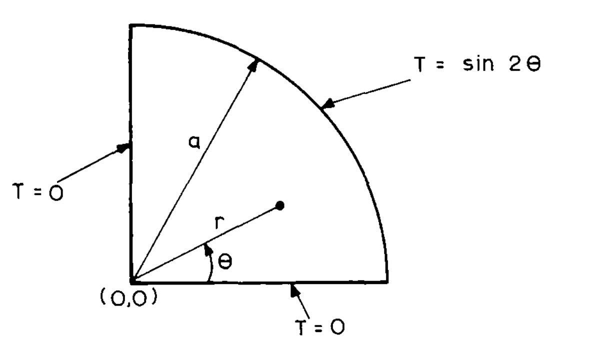

Fig. 2. Quarter cylinder co-ordinate system and boundary conditions

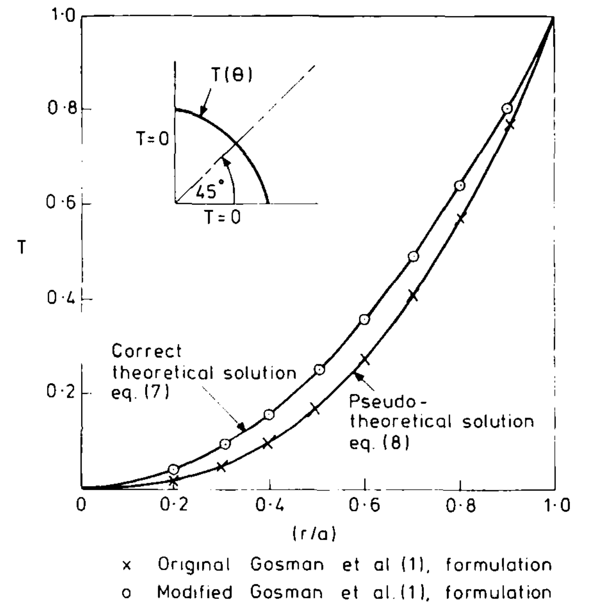

Fig. 3. Temperature distribution along bisector of a quarter cylinder

(b) Two-Dimensional Heat Conduction

Consider now the problem of finding the temperature distribution in a quadrant of an infinitely long cylinder of circular cross section (see Fig. 2). The governing equation for the temperature is

$$r^2 \frac{\partial^2 T}{\partial r^2} + r \frac{\partial T}{\partial r} + \frac{\partial^2 T}{\partial \theta^2} = 0 \qquad (6)$$

and with the boundary conditions shown this has the exact solution

$$T = \left(\frac{r}{a}\right)^2 \sin 2\theta \qquad (7)$$

The original Gosman *et al.* formulation, however, produces a solution of

$$r^2 \frac{\partial^2 T}{\partial r^2} + \frac{\partial^2 T}{\partial \theta^2} = 0$$

and hence should converge to

$$T = \left(\frac{r}{a}\right)^\alpha \sin 2\theta \qquad (8)$$

where $\alpha = (1 + \sqrt{17})/2$, and not to (7). The modified procedure is expected to converge to (7). These conclusions are amply borne out by reference to Fig. 3. The relative discrepancies between the modified and original formulations are most marked for small values of (r/a). It is interesting to note that these differences become even more pronounced if a full half cylinder is considered with $T = \sin \theta$ on the circular boundary or if any sector of the cylinder is considered with a constant non-zero temperature on the circular boundary.

CONCLUSIONS

A modification to the popular Gosman *et al.* (**1**) formulation for solving partial differential equations of the elliptic class has been proposed which renders the finite difference equations so derived compatible with the original differential equations for all geometries. The compatibility error in the Gosman *et al.* formulation has been shown to exist for all geometries for which either of the metric coefficients l_1 and l_2 are functions of the co-ordinates. It is therefore important to note that, for example, there is no incompatibility in the Gosman *et al.* finite difference equations when cartesian co-ordinates ($l_1 = l_2 = 1$) are used. The modifications, once seen, are obvious but have been tested successfully for two simple problems for which the original formulation was in error.

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