A NEW FINITE-VOLUME METHOD FOR CONVECTION-DIFFUSION PROBLEMS IN ARBITRARY TRIANGULATIONS

Axel E. Larreteguy
Centro Atómico Bariloche.
Comisión Nacional de Energía Atómica
8400 - S.C. de Bariloche, R.N., Argentina.

RESUMEN

El método de Volúmenes Finitos esta siendo aplicado desde hace años a la resolución de problemas de convección-difusión. Las funciones de forma lineales aparecen como inaplicables para números de Peclet moderados, por lo que ciertas funciones de forma particulares han sido propuestas por otros autores para superar esta dificultad. Se muestra en este trabajo que estas funciones dan lugar a aproximaciones fisicamente no realistas, además de tener un mal comportamiento numérico, cuando se aplican a elementos con ángulos obtusos.

Se propone una nueva función de forma que no adolece de las dificultades de las anteriores. Se presentan resultados teóricos y numéricos. Se puede concluir que el nuevo método produce aproximaciones realistas para cualquier forma de elemento, y muestra un muy buen comportamiento numérico. Puede trabajar con triangulaciones arbitrarias, haciendo mucho mas fácil la tarea de diseño de la red.

ABSTRACT

The Finite Volume Method has been applied for many years to the solution of convection-diffusion problems. Linear shape functions have proven to be inapplicable at even moderate Peclet numbers, and particular shape functions for triangular elements have been proposed by other authors to overcome this limitation. It is shown here that these functions lead to physically unrealistic approximations, and also have poor numerical behavior, when applied to elements with obtuse angles.

A new shape function that overcomes the aforementioned difficulties is proposed. Theoretical and numerical results are shown. It can be concluded that the new method produces realistic approximations whatever the shape of the elements, and shows a very good numerical behavior. It can handle successfully arbitrary triangulations, thus making very much easier the work of designing a grid.

INTRODUCTION

The purpose of this paper is to analyze and improve the Finite Volume Method (FVM), also called Control Volume based Finite Element Method (CVFEM) or BOX Method, as applied to the steady-state convection-diffusion equation.

The method, in its two-dimensional version as defined by Baliga and Patankar in [1], is based in domain discretization into 3-node triangular elements. A control volume is defined around each node of the mesh, as shown in Fig. 1. Each control volume is bounded by the lines joining the centroids of elements with the midpoints of their sides. This partition results in non-overlapping control volumes that extend over the complete calculation domain.

The discrete system of equations arises from a balance between the interior source and the flux crossing the surface of each control volume. To calculate these fluxes it is necessary to make some assumption concerning the shape of the unknown function v(x,y) within each element. This function should provide the value of v in the interior points of an element as a function of the values at the nodes. The values of v at these nodes are the unknowns to be obtained from the solution of the equations.

In this work the attention is focused on the properties and restrictions that certain shape functions produce in the FVM. A general theoretical frame that includes earlier shape functions is developed, and particular problems that occur with them are shown. Finally, a new shape function included in the aforementioned theoretical frame is proposed, that overcomes the difficulties found with the earlier ones.

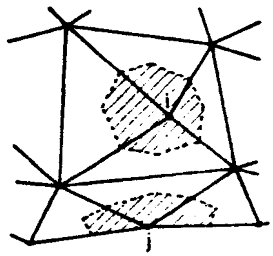

Fig. 1. Domain discretization.

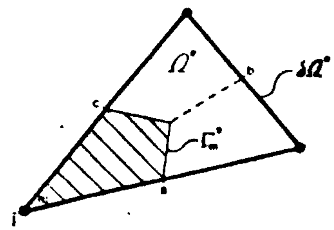

Fig. 2. An element and related notation

DEFINITION OF THE GRID AND RELATED NOTATION

The first step to obtain an algebraic approximation of the problem is to discretize the domain in triangular elements and to define control volumes surrounding each node, as shown in Fig. 1. In this figure two control volumes are shown, one surrounding an interior node (i) and the other a boundary node (j).
The interior of a control volume surrounding a generic node i will be called Ω_i and its surface $\delta\Omega_i$, with $\bar{\Omega}_i$ being the closure $\Omega_i \cup \delta\Omega_i$. The corresponding definitions for an element *e* will be denoted as Ω^e, $\delta\Omega^e$ and $\bar{\Omega}^e$. The volume Ω_i and its surface $\delta\Omega_i$ can be split into the elemental contributions

$$\Omega_i = \sum^e \Omega_i \cap \Omega^e = \sum^e \Delta^e_{im}\Omega^e_m \quad ; \quad \delta\Omega_i = \sum^e \delta\Omega_i \cap \Omega^e = \sum^e \Delta^e_{im}\Gamma^e_m \tag{1}$$

where the summation extends over all elements in the grid. The symbol Δ represents the connectivity matrix (Δ^e_{im}= 1 if the local node m of element e is the global node i, and is equal to 0 otherwise). The Eqs.(1) should be taken as a definition of Ω^e_m and Γ^e_m (see Fig.2). Einstein convention of summation over repeated indices is applied in this work, except for the supra-index e. The notation used in this paper was taken mainly from Chung [2].

THE FVM FOR THE STEADY-STATE CONVECTION-DIFFUSION EQUATION

Let us first review the FVM as applied to the solution of the well known 2-D general convection-diffusion equation (2)

$$\nabla \cdot \mathbf{j} = S \tag{2}$$

where

$$\mathbf{j} = \alpha\, \mathbf{u}\, v - \beta\, \nabla v \tag{3}$$

This equation determines the distribution of the scalar v, which is convected by a velocity field u and which diffuses according to Fick's Law where β stands for the diffusion coefficient. α is the convection coefficient and S is the volumetric rate of production of v, and will be called source. Eq.(2) appears in the modeling of heat, mass and momentum transfer.

After applying the Green-Gauss theorem to Eq.(2) written in integral form, the following equation is obtained.

$$\int_{\Gamma_i} j\cdot n \, d\Gamma = \int_{\Omega_i} S \, d\Omega \qquad (4)$$

The discretized system of equations is obtained by applying Eq.(4) to each node in the mesh. To evaluate the integrals in Eq.(4) it is necessary to know the variation of α, β, u, S and v over the whole domain. The parameters α, β and S are assumed constant within each element. The nodal values of u are known and a constant average value u^e is assumed within each element (linear interpolation was used in the works of Baliga and Patankar [1,3]).

The interpolation used for v inside an element e can be put in the following form:

$$v^e(x,y) = v^e_n \phi^e_n(x,y) \qquad ; \qquad n=1,3 \qquad (5)$$

These shape functions ϕ_n are the main objective of this paper, and will be considered in detail later.

When the shape functions of Eq.(5) are replaced in Eq.(4) an algebraic system of equations is obtained

$$A_{ij} \, v_j = b_i \qquad ; \; i,j=1,N \qquad (6)$$

where the global matrix A and vector b results of an assembling process of the following elemental ones

$$A^e_{mn} = \int_{\Gamma^e_m} (J^e_n \cdot n) \, d\Gamma \qquad ; \qquad J^e_n = (\alpha^e u^e \phi^e_n - \beta^e \nabla \phi^e_n) \qquad (7\text{-a})$$

$$b^e_m = \int_{\Omega^e_m} S^e \, d\Omega \qquad (7\text{-b})$$

Solving the system of Eq.(6), iteratively if the problem is non-linear, we obtain the desired values of v in each node.

EARLIER SHAPE FUNCTIONS - RESTRICTIONS AND DIFFICULTIES

The first shape functions ϕ_n used were obviously linear interpolations. This leads to algebraic systems similar to that obtained with the Galerkin approach in the Finite Element Method. Some error estimates for this method can be found in the paper of Bank and Rose [4].

It has long been known that the use of linear functions leads to oscillatory solutions for even moderate Peclet numbers (defined for the grid spacing), just like that observed with centered schemes in the Finite Difference Method.
To overcome this later difficulty Patankar and Baliga [1,3] have proposed the following interpolation inside each element (the upper-script e will be left off in this section for the sake of simplicity)

$$v(X,Y) = A \, W(X) + B \, Y + C \qquad (8)$$

where

$$W(X) = \Delta X \left[\frac{e^{(Pe \, X/\Delta X)} - 1}{e^{Pe} - 1} \right]$$

A local rotated system of coordinates X-Y is defined, so as to align the X axis with the average velocity u^e in the element, as shown in Figure 3. The parameter ΔX is the length of the element in direction X, the Peclet number (Pe) has been defined as

$$Pe = \alpha \, \| u^{*} \| \, \Delta X \, / \, \beta$$

It is important to note that

$$\lim_{Pe \to 0} W(X) = X$$

and then Eq.(8) leads to a linear interpolation in the pure diffusion case. Requiring that v should be coincident with the three nodal values v_m (m=1,3) in each element we can eliminate parameters A, B and C and rewrite Eq.(8) in the form of Eq.(5). In this case

$$\phi_m(X,Y) = a_m \, W(X) + b_m \, Y + c_m \qquad (9)$$

The nine constants a_m, b_m and c_m depend only on the values W_m=$W(X_m,Y_m)$ and Y_n at the three nodes. By defining three cyclic indices l, m and n (l,m,n=1,3) we can write

$$a_l = \frac{Y_n - Y_m}{\Delta} \; ; \quad b_l = \frac{W_m - W_n}{\Delta} \; ; \quad c_l = \frac{Y_n W_m - Y_m W_n}{\Delta} \qquad (10)$$

The determinant Δ is

$$\Delta = W_1 \, (Y_2 - Y_3) + W_2 \, (Y_3 - Y_1) + W_3 \, (Y_1 - Y_2) \qquad (11)$$

The functions of Eq.(9) were obtained as a suitable extension of the exact homogeneous one-dimensional case, but these functions lacks of an important property that their one-dimensional counterparts have. These two-dimensional functions can take values out of the range [0.,1.]. In fact they can take unbounded negative and positive values inside the element. Calling M the maximum absolute value of the three ϕ_m within the element we can make the following observation:

Observation 1: in certain conditions, if any of the three internal angles of the element is obtuse, there exists a finite Peclet number Pe^{*} for which $M \to \infty$ when $Pe \to Pe^{*}$. Proof: this observation can be easily demonstrated by means of a particular case. Consider the element shown in Fig.3. The value of Δ in this case is

$$\Delta = W_2 \, Y_3 - \Delta X \, Y_2$$

It should be noted that W_2 can take any value between X_2 (for Pe=0) and 0 (for $Pe \to \infty$), and therefore Δ will take values in the range

$$-\Delta X \, Y_2 \le \Delta \le \Delta X \, (Y_3 - Y_2)$$

and of course will take a null value for certain finite Pe^{*}. Following the definitions of Eq.(10)-(11), it is easy to see that the numerators of a_2, b_2 and c_2 are independent of Pe, and then these parameters can grow up without limit as $Pe \to Pe^{*}$. As a consequence, the value M in this example can also grow to infinity. This proves the observation.

The aforementioned observation shows the poor numerical behavior of these shape functions when dealing with obtuse angles. In this case the method is very likely to produce high roundoff errors. In addition, the resultant matrix has been observed to present values with very different orders of magnitude. This appears to be the cause of the slow convergence, due to high condition numbers, observed in the numerical experiments.

There is still another important difficulty. According to our numerical experience, a negative determinant Δ in an element produces negative diagonals in the matrix A for some or all of the control volumes that share that element. Following Patankar ([5], page 38) a method with such a behavior should not be accepted because it leads to physically unrealistic approximations. In elements with only acute angles, the determinant Δ can only have a null value for $Pe = \infty$, and therefore it never changes its sign. For this reason, the problem of negative diagonals does not arise if no obtuse angles are present in the mesh.

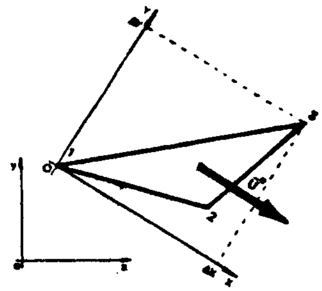

Fig. 3. Local coordinate system with X axis aligned with u^{e}.

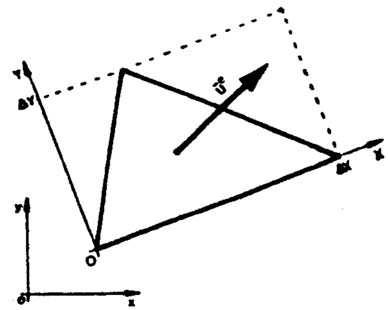

Fig. 4. Local coordinate system with X axis aligned with the largest side of the element.

Numerical results obtained with this functions in triangulations with obtuse angles will be presented later in this paper, showing clearly the effects of the above mentioned lost of physics realism.

NEW SHAPE FUNCTION PROPOSED

Suppose that the unknown field v can be expressed within an element as

$$v(x,y) = \xi(x) + \lambda(y) \tag{12}$$

If a condition of null divergence is impossed on the resulting flux j, the following relation is obtained

$$\nabla \cdot [\alpha u(\xi+\lambda) - \beta \nabla(\xi+\lambda)] = 0 \tag{13}$$

If α, β and $u=(u_x, u_y)$ are assumed constant inside the element and specifying that Eq.(13) must hold for the two functions ξ and λ separately, the following relations are obtained:

$$\alpha\, u_x \frac{\partial \xi}{\partial x} - \beta \frac{\partial^2 \xi}{\partial x^2} = 0 \quad ; \qquad \alpha\, u_y \frac{\partial \lambda}{\partial y} - \beta \frac{\partial^2 \lambda}{\partial y^2} = 0 \tag{14}$$

The general solutions of Eq.(14) are

$$\xi(x) = A\, W(x) + C_x \quad ; \qquad \lambda(y) = B\, Z(y) + C_y \tag{15}$$

where

$$W(x) = \Delta x \left[\frac{e^{(Pe_x\, x/\Delta x)} - 1}{e^{Pe} - 1} \right] \quad ; \quad Z(y) = \Delta y \left[\frac{e^{(Pe_y\, y/\Delta y)} - 1}{e^{Pe} - 1} \right]$$

This modified Peclet numbers can take either sign and are defined as

$$Pe_x = \alpha\, u_x\, \Delta x / \beta \quad ; \quad Pe_y = \alpha\, u_y\, \Delta y / \beta$$

Repeating what has been done in the last section we can write the three nodal shape functions as

$$\phi_n(x,y) = a_n\, W(x) + b_n\, Z(y) + c_n \tag{16}$$

where

$$a_1 = \frac{Z_2 - Z_3}{\Delta} \quad ; \qquad b_1 = \frac{W_3 - W_2}{\Delta} \quad ; \quad c_1 = \frac{Z_3 W_2 - Z_2 W_3}{\Delta} \tag{17}$$

The determinant Δ is now

$$\Delta = W_1 (Z_2-Z_3) + W_2 (Z_3-Z_1) + W_3 (Z_1-Z_2) \qquad (18)$$

Another approach that leads to two exponential shape functions, although in structured grids of square elements, can be found in the work of O'Riordan and Stynes [6].

The function proposed so far still have the same problems as that of Patankar. Consider again the case of Fig.3. If Pe_y is 0. the new shape function reduces to that of Eq.(9) , and of course presents the same problems. It should be noticed, however, that the new proposition does not require any rotation imposed by the local flow field, so we are free to define it for any rotated (or not) system X-Y. The key idea of the method proposed is to choose a particular rotation that results in shape functions with excellent numerical behavior.

Consider the element of Fig.4. The rotated system X-Y has been chosen so as to align the X axis with the largest side. If we now construct our functions of Eq.(16) in this system, the following observation can be made:

Observation 2: The maximum absolute value M of the functions ϕ_n (n=1,3) in $\bar{\Omega}^e$ is equal to 1 always.
Proof: the definition of Δ of Eq.(18) applied to this particular rotation gives $\Delta = \Delta X\ \Delta Y$ always (it is independent of the values of Pe_x and Pe_y). Using Eq.(17) we can rearrange Eq.(16) in the following form

$$\phi_1(X,Y) = [\ W(X)\ (Y_2-Y_3) + W_2\ (Y_3-Y) + W_3\ (Y-Y_2)\ ] / \Delta$$

$$\phi_2(X,Y) = [\ W_1\ (Y-Y_3) + W(X)\ (Y_3-Y_1) + W_3\ (Y_1-Y)\ ] / \Delta$$

$$\phi_3(X,Y) = [\ W_1\ (Y_2-Y) + W_2\ (Y-Y_1) + W(X)\ (Y_1-Y_2)\ ] / \Delta$$

It is easy to see from elementary geometry that
■ i) an expression like

$$x_a\ (y_b-y_c) + x_b\ (y_c-y_a) + x_c\ (y_a-y_b)$$

represents, in module, twice the area of the triangle abc (this value can be positive or negative depending on the orientation of the three points).
■ ii) if the triangle is enclosed in a box, so that $0 \le x \le \Delta x$ and $0 \le y \le \Delta y$, then the maximum possible area for such a triangle is $\Delta x \Delta y/2$.

From the two above mentioned properties of triangles and the form of the rearranged expressions of ϕ_n, recalling that $0 \le W(X) \le \Delta X$ and $0 \le Z(Y) \le \Delta Y$, it is clearly seen that the three functions ϕ_n always take values in the range [-1,1] within the element, that is to say

$$-1 \le \phi_n(X,Y) \le 1$$

As they take the value 1 at least in the corresponding node it follows that M=1 and therefore observation 2 is true.

The method proposed then consists in using the functions defined in Eq.(16) in a system locally rotated so as to align the X axis with the largest side of the triangle. This method has the following main advantages:

i) the determinant Δ has a constant positive value. No negative diagonals are allowed to arise thus ensuring physically realistic approximations under all circumstances.

ii) the condition number of the resultant matrix shows great improvements when compared with earlier methods.

iii) the new proposed method is not likely to show high roundoff errors because the values of the shape functions are restricted to the range [-1,1] inside $\bar{\Omega}^e$.

In the next sections numerical results and comparisons with earlier methods are shown.

NUMERICAL RESULTS AND COMPARISONS

To provide experimental support to the theoretical results of the precedingsections some numerical results and comparisons will be shown. To carry out the calculations shown in this section, a computer code was set up. Sparse matrix techniques [7] were used, in order to obtain a code capable of handling large problems and arbitrary unstructured meshes. Because direct solution by Gaussian elimination becomes extremely slow, or inapplicable at all, in medium to large problems with non-symmetric matrices, a conjugate-gradient-like method called Conjugate Gradient Squared (CGS) [8] was implemented. An incomplete LU decomposition (ILU) method (Kershaw [9,10]) was used successfully as a preconditioner. Using the aforementioned code two problems, enough to show the advantages of the proposed method, were considered. The first is an academic benchmark and the second is a real technologic problem.

Problem 1:
This is a well known benchmark taken from Glowinsky [11]. Consider the domain Ω shown in Fig.5. An uniform velocity field $u=(1,0)$ and a constant source $S=1$ are imposed over it. A constant temperature $T=0$ is given over the whole boundary $\partial\Omega$.

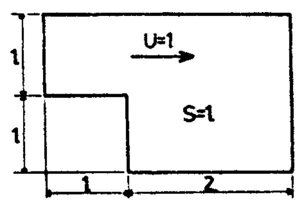

Fig. 5. Problem 1: Domain and boundary conditions.

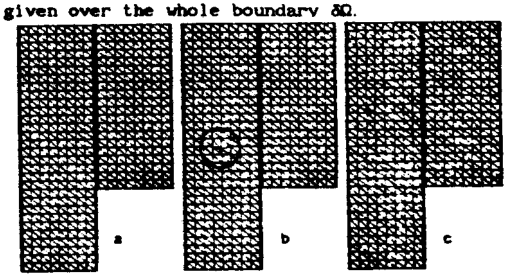

Fig. 6. Problem 1: Grids.

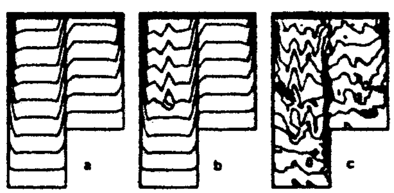

Fig. 7. Problem 1: Earlier method

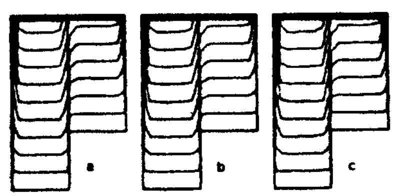

Fig. 8. Problem 1: Proposed method.

Numerical results of this problem with $\alpha=1.$ and $\nu=0.001$ were obtained using the three grids shown in Fig.6. They all have 1000 elements and 561 nodes. The grid shown in Fig.6-a has horizontal bands of refined elements to avoid wiggles of temperature in the boundary layers for high Peclet numbers. The grid of Fig.6-b is equal to that of Fig.6-a except for a single node that was moved up and left in order to produce an element with an obtuse angle. The grid shown in Fig.6-c is that of Fig.6-a with all but the boundary nodes moved in random directions a fixed small distance (0.01), producing randomly distributed slightly distorted elements, some of them with obtuse angles.

The solutions obtained using the function proposed by Baliga and Patankar in the three grids are shown in Fig.7. In this figure 11 isothermal lines, evenly distributed from 0. to 3., are shown. The distortion of a single node has produced a negative diagonal on the corresponding row of the matrix, thus given an unrealistic temperature peak transported downstream by the velocity field. The Fig.7-c shows clearly a totally distorted solution obtained with the randomly modified grid. In this case 134 negative diagonals where detected in matrix A.

The results obtained with the new proposed functions for the three grids are shown in Fig.8. It is clearly seen that the solution was not affected at all in the case of Fig. 8-b and only small disturbances appear in Fig.8-c. No negative diagonals were detected.

Another important effect to be taken into account is the improvement in the condition number of matrix A. The problem of grid 6-a was solved in 13 CGS iterations with both methods. The problem of grid 6-c was also solved in 13 CGS iterations with the new method, but it took 110 iterations to obtain a converged solution when the method of Baliga and Patankar was applied.

Problem 2:
This is a real case of a thermal problem that appears in a coextrusion process of two distinct materials [12]. The details of this problem are not relevant for us. The velocity field and the nonuniform heat source, due to internal friction, have been taken from a Finite Element solution of the dynamic problem. The boundary conditions, with temperatures normalized to 0. at the inlet, are shown in Fig.9. The streamlines of the velecity field and the grid used are shown in Figs. 10 and 11.

Two cases, with different diffusivities, are considered.

i) The highest Peclet grid number is in this case about 5000. The real diffusivity of the problem has been artificially increased in order to compare numerical results. It was impossible to obtain converged solutions with the earlier method of Eq.(9) for diffusivities lower than that used in this case. The solutions obtained with the method of Eq.(9) and the proposed method are compared in Fig.12 and 13. The earlier method shows negative temperatures ($-3.<T<4.$), which are completely unrealistic because of the boundary conditions and the fact that the heat source is positive everywhere. With this method, 34 negative diagonals where detected in the matrix. In Fig.15, the plots of the residual versus CGS iterations are shown. The improvement in the rate of convergence obtained with the new proposed method is clearly seen.

ii) The diffusivity has been given a value 5 times lower than that of the preceding case. As has been said before, only the solution obtained with the new proposed method can be shown in Fig.14. With the earlier method, 153 negative diagonals were detected and a converged solution was imposible to be obtained. The converge behavior of the two methods are compared in Fig.16.

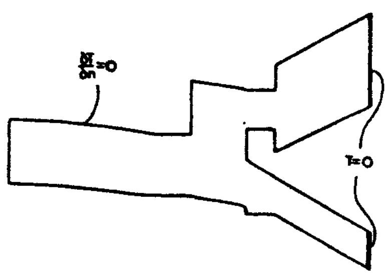

Fig. 9. Problem 2: Domain and boundary conditions

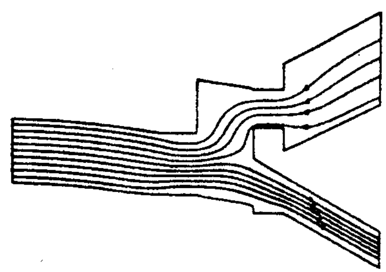

Fig. 10. Problem 2: Given streamlines.

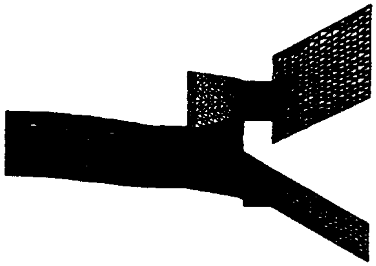

Fig. 11. Problem 2: Grid.

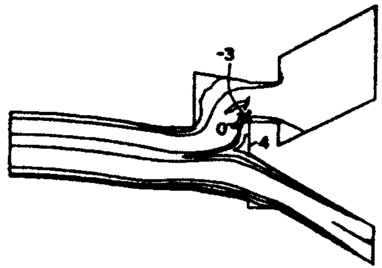

Fig. 12. Problem 2: Case i.
Earlier method.

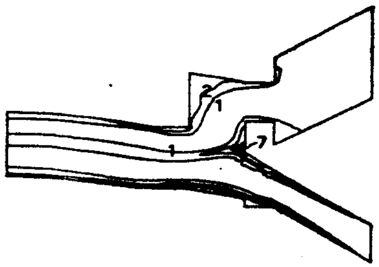

Fig. 13. Problem 2: Case i.
Proposed method.

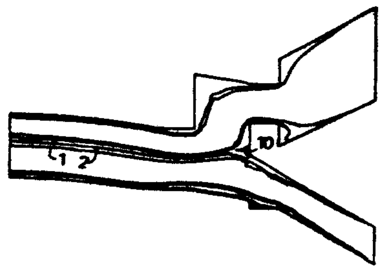

Fig. 14. Problem 2: Case ii.
Proposed method.

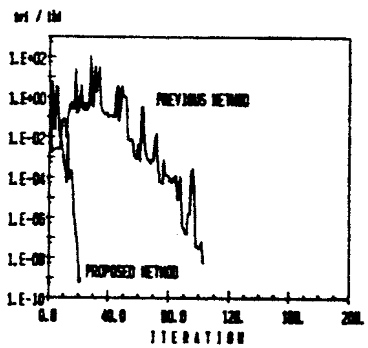

Fig. 15. Problem 2: Case i.
Plots of residuals.

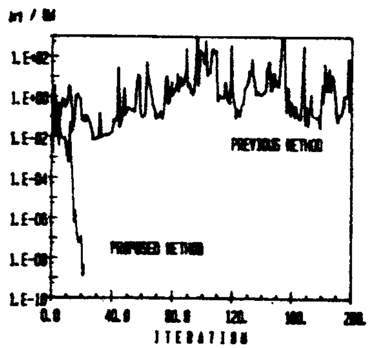

Fig. 16. Problem 2: Case ii.
Plots of residuals.

CONCLUSIONS

A new Finite Volume Method for solving convection-diffusion problems has been proposed. A new shape function, that includes earlier propositions of other authors as a particular case, has been introduced. The better numerical behavior of the new shape function has been both theoretically and numerically proved.

In our numerical experiments, two of which have been shown here, the new method has consistently presented three main advantages when compared with earlier propositions:
i) No negative diagonals are allowed to arise in the matrix whatever the shape of the elements. This ensures physics realism to be maintained.
ii) The condition number of the resultant matrix appears to be greatly improved, showing considerably lower solving times.
iii) High roundoff errors are not likely to be produced because the values of the shape functions are restricted always to the range [-1,1].
As a final conclusion it can be said that the new method produces faster and very robust codes, allowing also great flexibility in the design of the grids.

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