EFFECTS OF TREATMENT OF SOURCE TERMS IN TURBULENT MODELS ON CONVERGENCE RATE

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Abstract

After substantial progress has been made in solving flow field accurately, the robustness of a numerical scheme has raised growing interest in CFD community. Solution of turbulence model equations poses additional difficulties compared with the solution of mean-flow equations. Method to ensure the discrete positivity of turbulence eddy viscosity is proposed by Baldwin & Barth and later expanded by Spalart & Allmaras in the solution of their respective one-equation turbulence models.

It is noticed during the current research that the strategy proposed by Spalart and Allmaras is a sufficient but unnecessarily restrictive condition for the solution procedure to be positively conservative, and that there is no fundamental reason to split the Jacobian of the combined source term into two parts. The presence of the temporal term allows more information from the exact Jacobian of the combined source term to be extracted. A new strategy of treatment of source terms, having the potential to give even better convergence characteristic, is proposed. In addition, previous works have been restricted to first-order accurate discretization of convection terms in the turbulence model. A way to extend the positivity property to second-order accurate discretization of convection terms is proposed.

1 Introduction

After substantial progress has been made in the effort of seeking *accurate* numerical schemes for capturing shock and contact discontinuities with minimal dissipation and oscillations, the *robustness* of numerical schemes has raised growing interest in CFD community, especially in the conservative computation of flows containing regions in which the total energy is overwhelmingly dominated by the kinetic energy mode. A new concept, the so-called positivity property of a numerical scheme, has been proposed to describe one mathematical aspect of scheme robustness. A scheme is said to be positively conservative if, starting from a set of physically admissible states, it can only compute new states with positive values. Method to extend one-dimensional first order accurate positively conservative numerical flux schemes to more dimensions and higher order was proposed in [1]. A CFL-like condition to ensure the positivity property of flux vector splitting (FVS) schemes is derived in [2].

Solutions of turbulence model equations poses additional difficulties either because of the presence of strong source terms, which will introduce additional time scale s and thereby causing the stiffness problem, or because of the singular behavior of the modeled turbulent quantities near solid boundaries, or because of non-analytical behavior at sharp turbulent-nonturbulent interface [3]. Even though turbulent quantities such as k, ω, ε, μ_T, etc, should remain positive on physical basis, and the exact solution of the model equations can often be shown to be strictly non-negative, inappropriate discretization and resolution of the model equations may generate negative values. Besides being unphysical, negative values of the eddy viscosity cause back-scatter of energy from turbulence to mean flow, a process not even considered in the eddy-viscosity type of turbulence models. It in turn could lead to a rapid explosion of the solution of turbulence-model and mean-flow equations. This is most likely to occur in the initial transient phase when initial values for both mean-flow and turbulent variables are far from converged physical solutions. When the problem occurs, it can usually be postponed or avoided by lowering the time-step, resetting the negative value to a small positive value, discretizing convection terms with first order accurate scheme, or imposing some limitation on the allowable level of production source terms. However, what one needs is a scheme that preserves positivity for all time, without excessively degrading the accuracy and convergence rate.

In [4], discrete positivity of the turbulence eddy viscosity in the solution of Baldwin-Barth's one-equation model is ensured through the use of positive discrete operator and M-type matrices. A positive operator is one that maps a vector with nonnegative components into a vector with nonnegative components. An M-type matrix is diagonally dominant with positive diagonal elements and non-positive off-diagonal elements. In addition, it must be either strictly diagonally dominant or else irreducible and diagonally dominant with strict diagonal dominance for at least one row. An important property of an M-type matrix is that all elements of its inverse are non-negative; thus the inverse of an M-type matrix is a positive operator. In [5], Baldwin & Barth's approach for the solution of turbulence transport model is expanded, and several ways of treatment of source terms in the solution of Spalart-Allmaras's one-equation turbulence model are compared. A new strategy is identified as being both robust and efficient. In [6], similar approach is extended to the solution of Spalart-Allmaras's one-equation turbulence model equation on unstructured grids.

It is noticed during the current research that the strategy proposed by Spalart and Allmaras is a sufficient but unnecessarily restrictive condition for the solution procedure to be positively conservative. The presence of the temporal term allows more information from the exact Jacobian of the combined source term to be extracted. A new strategy of treatment of source terms, expected to give even better convergence characteristic, is proposed. In addition, previous works have been restricted to first-order accurate discretization of convection terms in the turbulence model, and it is not obvious under what conditions a second-order accurate discretization can be guaranteed to remain positively conservative. The determination of such conditions is another goal of the present paper.

The paper is organized as follows. In section 2, Spalart-Allmaras's strategy in the solution of their one-equation turbulence model will be briefly described. In section 3, a new strategy for the treatment of source terms will be proposed and its effect on convergence rate tested against a simple case. In section 4, extension of positivity property to second order accurate discretization of convection terms will be proposed and tested. In section 5, a note on the resolution of the discretized model equation will be given. Finally, the works done in this paper will be summarized and future work outlined.

2 Spalart-Allmaras's Strategy in the Solution of Their Turbulence Model

The Spalart-Allmaras model is a relatively recent eddy viscosity model based on a single transport equation for a variable related to the turbulent viscosity. This model was inspired from an earlier model developed by Baldwin and Barth. Its formulation and coefficients were defined using dimensional analysis, Galilean invariance, and selected empirical results, such as two-dimensional mixing layers, wakes, and flat-plate boundary layer flows. The model gives improved predictions obtained with algebraic mixing-length models for complex flows, and provides a simpler alternative to two-equation turbulence models. The model does not give good predictions in jet flows, but gives reasonably good predictions of 2-D mixing layers, wake flow, and flat-plate boundary layers and shows improvements in the prediction of flows with adverse pressure gradients compared with the k-ε and k-ω models, although not as much as the k-ωSST model [7]. The modeled variable behaves linearly near the solid wall. It does not require as fine a grid resolution in wall-bounded flows as two-equation turbulence models and has shown convergence behavior comparable to or even better than algebraic models.

The transport equation for a turbulence quantity, related to eddy viscosity via an algebraic equation, in Spalart-Allmaras's one-equation turbulence model reads:

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = \frac{1}{\sigma}\left[\frac{\partial}{\partial x_j}\left((\nu+\tilde{\nu})\frac{\partial \tilde{\nu}}{\partial x_j}\right) + c_{b2}\left(\frac{\partial \tilde{\nu}}{\partial x_j}\right)^2\right] + c_{b1}(1-f_{t2})\tilde{S}\tilde{\nu} - \left(c_{w1} f_w - \frac{c_{b1}}{\kappa^2} f_{t2}\right)\left(\frac{\tilde{\nu}}{d}\right)^2 + f_{t1}\Delta U^2 \quad (1)$$

where $\tilde{\nu}$ represents the modeled turbulent quantity, u is velocity, t is time, x is the coordinates. For the meaning of other variables in the equation, please refer to the original paper [5].

Equation (1) can be rewritten in a form more convenient for numerical analysis:

$$\frac{\partial \tilde{\nu}}{\partial t} + u_j \frac{\partial \tilde{\nu}}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\lambda \frac{\partial \tilde{\nu}}{\partial x_j}\right) + P(\tilde{\nu})\tilde{\nu} - D(\tilde{\nu})\tilde{\nu} \quad (2)$$

where λ signifies general diffusion coefficient. Note the source terms are written in a special form to facilitate numerical analysis.

Equation (2) can be integrated in time using an implicit backward-Euler scheme of the form:

$$\left[I - \Delta t(\overline{J_C} + \overline{J_{Diff}} + \overline{J_{S_P}} - \overline{J_{S_D}})\right]\Delta\tilde{\nu}^n = \Delta t\left[C + Diff + P - D\right]\tilde{\nu}^n \quad (3)$$

where $\overline{J_C}$, $\overline{J_{Diff}}$, $\overline{J_{S_P}}$ *and* $\overline{J_{S_D}}$ are the discrete approximate Jacobians of the convection, diffusion, production and destruction terms respectively; Δt is time step; and $\Delta\tilde{\nu}$ is solution change.

Rearrangement of (3) gives $\tilde{\nu}^{n+1}$ directly as a function of $\tilde{\nu}^n$:

$$[I - \Delta t(\overline{J_C} + \overline{J_{Diff}} + \overline{J_{S_p}} - \overline{J_{S_D}})]\tilde{\nu}^{n+1} = [I + \Delta t(C + Diff + P - D) - \Delta t(\overline{J_C} + \overline{J_{Diff}} + \overline{J_{S_p}} - \overline{J_{S_D}})]\tilde{\nu}^n \quad (4)$$

Assuming that $\tilde{\nu}^n$ is non-negative, then non-negativity of $\tilde{\nu}^{n+1}$ is guaranteed if the right -hand-side (RHS) operator is positive and left-hand-side (LHS) operator forms an M-type matrix. It is shown is [5] that the first-order accurate discretization of the convection terms and second-order central differencing of the diffusion terms will form M-type matrix components at LHS and positive operator components at RHS.

Turbulent transport equations differ from the mean-flow governing equations in their presence of strong source terms, which may dominate the budget of the equation in some regions of the field. Inappropriate treatment of the source terms may lead to the violation of the diagonal dominance of the LHS matrix of the resultant system of algebraic equations, and in turn resulting in negative turbulent viscosity and causing divergence of the solution. In common practice, the production terms are treated explicitly (lagged in time) while destruction terms are treated implicitly (they are linearized and a term is brought to the LHS of the equations which helps to increase the diagonal dominance of the LHS matrix). While this strategy proves to be numerically highly stable, the convergence rate is not as satisfactory. In regions where both production and destruction are large and dominate the equation budget, this strategy can result in extremely slow convergence, as the Jacobians of production terms and destruction terms in these regions will be individually large but will tend to cancel. If only Jacobian of the destruction terms are used to update the solution, the contribution to the diagonal element of the matrix will be excessive, the resulting solution change will be correspondingly small even when the residuals are not close to zero. Realizing this possible cancellation of the individually large Jacobians, Spalart and Allmaras proposed to treat the source terms combined together, splitting the Jacobian of the combined term into two terms, and then extracting the negative part of each term and moving them to the LHS.

The approximate Jacobian for source terms proposed by Spalart and Allmaras is taken as:

$$\overline{J_{S_P}} - \overline{J_{S_D}} = neg(P-D) + neg(P' - D')\tilde{\nu} \qquad (5)$$

where

$$neg(x) = \begin{cases} 0 & if \quad x \geq 0 \\ x & if \quad x < 0 \end{cases} \qquad (6)$$

This strategy maintains M-type matrix at LHS, and positive operator at the RHS of equation (4). Hence the non-negativity of the turbulence quantity during the solution process is guaranteed. In addition, due to the combined treatment of the source term, the convergence rate is also enhanced.

3 A New Strategy in the Treatment of Source Terms

Newton's method, with exact Jacobians being used, is a powerful iterative solution method for nonlinear equations for it could give quadratic convergence rate in the neighborhood of the root. When approximate Jacobians have to be used, they should be as close to the exact ones as possible to achieve near-quadratic convergence rate. In the solution of turbulence model equations, however, exact Jacobians of source terms may violate the diagonal dominance of the iterative matrix at LHS, destroy the positivity of solution, and cause solution divergence.

Spalart and Allmaras has found an effective way of forming an approximate Jacobian of the combined source terms which closely resemble the exact Jacobians while not violating the diagonal dominance of the iterative matrix at LHS. Improved convergence behavior is obtained. Nevertheless, it has to be pointed that, while treating both the production and destruction source terms as combined together is appropriate, there is no fundamental reason to split the Jacobian of the combined source term into two parts. Furthermore, the condition on the source term Jacobians (equation (5)) to maintain non-negativity of the turbulent quantity is sufficient but not unnecessarily restrictive. It is hoped that the convergence rate may be further improved by deriving a less restrictive condition and keeping the Jacobian of the combined source term as unsplit.

It is noticed that the presence of the temporal term, always producing positive valued diagonal entries on both side of the discretized equation and thereby enhancing diagonal dominance at LHS and maintaining positive operator at RHS, allows more information from the exact Jacobian of the combined source term to be extracted and brought to the LHS. A new strategy of treatment of source terms, expected to give even better convergence characteristic, can be formulated by exploiting this extra freedom.

With backward Euler discretization of temporal term, first order accurate discretization of convective terms and second order accurate discretization of diffusion terms remain unchanged, the necessary and sufficient conditions for the maintenance of M-type matrix on the LHS and positive operator on the RHS of equation (4) is:

$$\begin{cases} I - \Delta t \overline{J_S} > 0 \\ I + \Delta t (P - D - \overline{J_S}) > 0 \end{cases} \qquad (7)$$

where $\overline{J_S} = \overline{J_{S_P}} - \overline{J_{S_D}}$, is approximate Jacobian of source terms as combined together.

Therefore, approximate Jacobian of source terms can be determined as:

$$\begin{cases} \overline{J_S} < \dfrac{I}{\Delta t} \\ \overline{J_S} < \dfrac{I}{\Delta t} + P - D \end{cases} \qquad (8)$$

In condition (5), only when either part of the source Jacobians is negative, is it included in the approximate Jacobian. In condition (8), the unsplit Jacobian of combined source term could be positive. It is included into the approximate Jacobian as long as it is bounded by two upper limits, which could be of large magnitude. The approximate Jacobian is set to the lower one of the bounds if the exact Jacobian exceeds them. Therefore, the resultant approximate Jacobian of the source term will resemble the true Jacobian to a greater extent, which will help to achieve faster convergence rate.

To compare the effect of these two conditions on the convergence rate, flow over flat plate is chosen as a test problem. The inflow Mach number is 2. The Reynolds number based on the flat plate length is 10^7. Initial values for $\tilde{\nu}$ is set to 1.34 at inflow, and a small positive number elsewhere. Fig 1 shows the predicted law of wall against an empirical formula. There is essentially no difference between the convergence solutions.

The convergence history of the absolute norm of the residual, relative to the initial value, for three different treatments of source terms, is shown in Fig 2. Spallart-Allmaras's strategy gave slightly faster convergence than that of common practice. The new strategy proposed in this paper converged slightly faster than that of Spallart-Allmaras's at the initial stage.

The reason for this apparent indifference of convergence rate to the treatment of source terms become clear by inspecting Fig 3, which shows the budget of $\tilde{\nu}$ at a typical location across boundary layer, and Fig 4, which shows approximate Jacobians resulted from the three different treatments. It is clear that in this simple flat plate flow, the dissipation term dominates production term in most part of the boundary layer, therefore, all the three strategies give rise to essentially same approximate Jacobians.

The strength of the proposed strategy is expected to be fully realized in the computation of more complex flow with adverse pressure gradient, where the production term will become significant and dominating.

4 Extension to Second Order Accurate Discretization of Convection Terms

As noted in introduction, previous works in positively conservative solution of one-equation turbulence model have been restricted to first-order accurate discretization of convection terms of the model equation. And it is not obvious under what conditions a second-order accurate discretization can be guaranteed to remain positively conservative, as a straightforward extension will certainly destroy the diagonal dominance of, as well as introducing positive entries into, the LHS matrix, thereby invalidating it as an M-type matrix. The author found that the desirable positivity property could be extended to second-order accurate discretization of convection terms with a different treatment of convection terms on two sides of the discretized equation and a proper limitation on local time step.

The convection terms at new time step are split into a contribution from previous time step and an increment, with the former part discretized second order accurately and the latter part first order accurately:

$$
\begin{aligned}
u_j \frac{\partial \tilde{\nu}^{n+1}}{\partial x_j} &= u_j \frac{\partial(\tilde{\nu}^n + \Delta\tilde{\nu}^n)}{\partial x_j} \\
&= u_j \left.\frac{\partial \tilde{\nu}^n}{\partial x_j}\right|_{2nd} + u_j \left.\frac{\partial \Delta\tilde{\nu}^n}{\partial x_j}\right|_{1st} \\
&= u_j \left.\frac{\partial \tilde{\nu}^n}{\partial x_j}\right|_{2nd} - u_j \left.\frac{\partial \tilde{\nu}^n}{\partial x_j}\right|_{1st} + u_j \left.\frac{\partial \tilde{\nu}^{n+1}}{\partial x_j}\right|_{1st} \\
&\equiv (C_{2nd}^n - C_{1st}^n) + u_j \left.\frac{\partial \tilde{\nu}^{n+1}}{\partial x_j}\right|_{1st}
\end{aligned}
\tag{9}
$$

With backward Euler discretization of temporal term, second order accurate discretization of diffusion terms, the necessary and sufficient conditions to maintain M-type matrix on the LHS and positive operator on the RHS of equation (4) is:

$$
\begin{cases}
I - \Delta t \overline{J_S} > 0 \\
\tilde{\nu}^n + \Delta t (P - D - \overline{J_S})\tilde{\nu}^n - \Delta t (C_{2nd}^n - C_{1st}^n) > 0
\end{cases}
\tag{10}
$$

Here two alternative treatment of the source Jacobians are possible, which will lead to different restriction of allowable time step. The first alternative is to use the strategy proposed by Spalart and Allmaras, where the above restrictions can be relaxed and reduced to:

$$\Delta t < \frac{\tilde{\nu}^n}{C_{2nd}^n - C_{1st}^n} \quad if \quad C_{2nd}^n - C_{1st}^n > 0 \tag{11}$$

The second alternative is to use exact Jacobian of combined source term, which will impose a stricter restriction of allowable time step:

$$\begin{cases} \Delta t < \dfrac{I}{J_S} & if \quad J_S > 0 \\ \Delta t < \dfrac{\tilde{\nu}^n}{(P' - D')\tilde{\nu}^n + (C_{2nd}^n - C_{1st}^n)} & if \quad denominator > 0 \end{cases} \tag{12}$$

While both alternatives could guarantee the positivity of solution, their respective effects on the convergence rate is not entirely obvious. On one hand, the use of the exact source Jacobian might enhance convergence; on the other hand, stricter restriction of local time step will inhibit convergence. The final conclusion can only be drawn after extensive application to various flow problems.

Fig 5 shows the convergence history of relative residual with second order accurate discretization of convection terms and with two different restrictions on time step according to equation (11) and (12). Essentially same convergence rate is exhibited.

5 A Note on the Resolution of the Discretized Equation

In principle, solving Reynolds-averaged Navier-Stokes equations and turbulence-model equation as coupled together may have better convergence behavior. However, the coupling between mean-flow and turbulence-model equations seems to be relatively weak. So far, limited experience appears to indicate there is no appreciable gain to solve all equations simultaneously as opposed to solving them sequentially. In common practice the mean-flow and turbulence-model equations are solved sequentially, with the primary coupling through eddy viscosity. In the case of two-equation turbulence models, the two model equations are also solved decoupled from each other. This approach allows different discretization schemes, different time steps, and different solution methods, to be applied as appropriate. In addition, it facilitates the incorporation of different turbulence models.

It has to be noted that previous argument about the positivity property of numerical method assumes that the discretized model equation is solved exactly. This is unnecessarily expensive, as in the time marching to steady state, the intermediate states are physically irrelevant and an approximate resolution with a certain level accuracy will give an overall better convergence behavior. That is, some compromise has to be made between absolute robustness and ultimate efficiency. In [5], the discretized model equation is solved with approximate factorization, the factorization error being reduced through subiterations. In [6], the equation is solved with Gauss-Seidel procedure with 15 subiterations, and if updated eddy-viscosity does turn negative, it is reset to freestream value. The present paper solved the discretized model equation with alternating-direction-implicit (ADI). One back-and-forth and up-and-down sweep was enough to drive the residual to acceptably low level.

6 Summary

After substantial progress has been made in solving flow field accurately, the robustness of numerical schemes has raised growing interest in CFD community. Solution of turbulence model equations poses additional difficulties compared with the solution of mean-flow equations. Method to ensure the discrete positivity of turbulence eddy viscosity is proposed by Baldwin & Barth and later expanded by Spalart & Allmaras in the solution of their respective one-equation turbulence models.

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Two-equation turbulence models pose much more severe numerical difficulties than that by Spalart-Allmaras's one-equation model. The substantial gain in the robustness and convergence rate through the use of M-type matrix and positive operator in the solution of one-equation model encourages future effort to extend the same idea to the solution of two-equation turbulence models.

References

[1] Linde T and Roe P. L. On multidimensional positively conservative high-resolution schemes, Barriers and Challenges in Computational Fluid Dynamics, pp299-313, Kluwer Academic Publishers, 1998.

[2] Gressier J, Villedieu P and Moschetta J.M. Positivity of flux vector splitting schemes, Journal of Computational Physics, Vol. 155, pp199-220, 1999

[3] Wilcox D.C. Turbulence modeling for CFD, DCW Industries, Inc. pp273-313, 1994.

[4] Baldwin, B. and Barth, T. A One-Equation Turbulent Transport Model for High Reynolds Number Wall-Bounded Flows, NASA TM-102847, August 1990.

[5] Spalart, P and Allmaras, S. A One-Equation Turbulence Model for Aerodynamic Flows, AIAA paper, 92-0439,1992

[6] Ashford G.A. and Powell K.G. An unstructured grid generation and adaptive solution technique for high-Reynolds-number compressible flows, von Karman Institute for Fluid Dynamics, Lecture Series 1996-06.

[7] Bardina J.E. Huang P.G. and Coakley T.J. Turbulence modeling validation, testing, and development, NASA TM-110446, 1997.

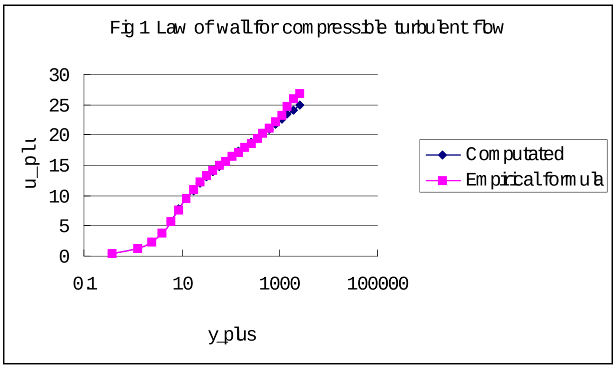

Fig 1 Law of wall for compressible turbulent flow

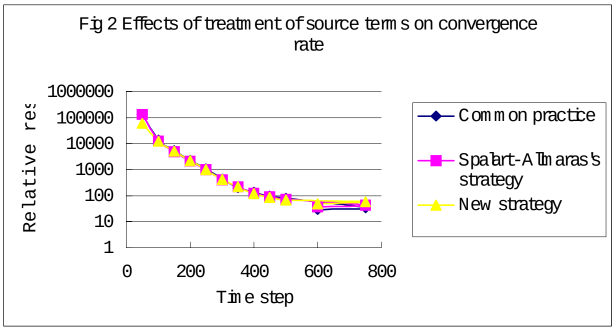

Fig 2 Effects of treatment of source terms on convergence rate

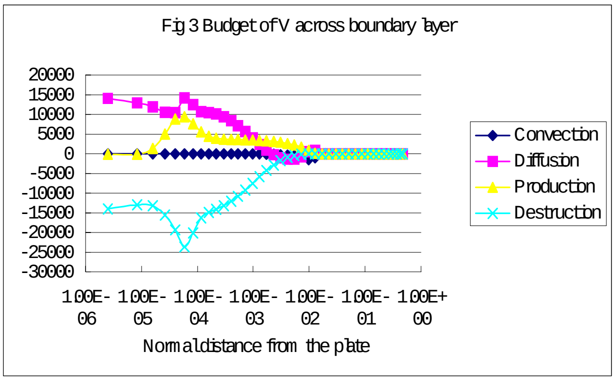

Fig 3 Budget of V across boundary layer

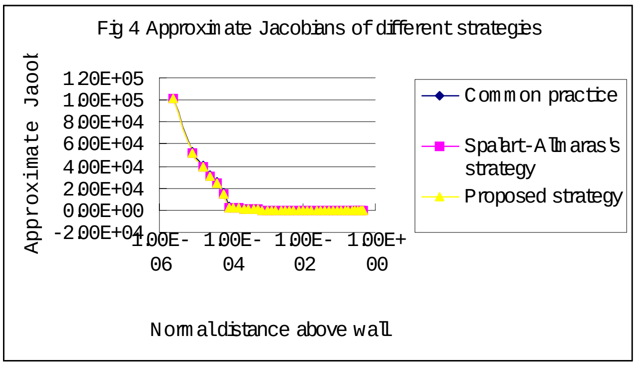

Fig 4 Approximate Jacobians of different strategies

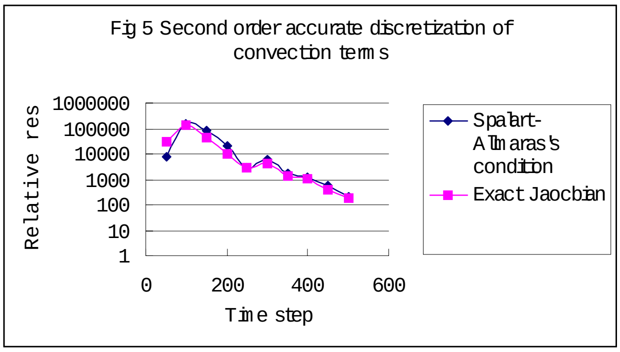

Fig 5 Second order accurate discretization of convection terms