106 KSME International Journal, Vol. 11, No. 1, pp. 106 ~ 114, 1997

A Convection Scheme Sensitized to the Convection Direction of a Scalar Quantity

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(Received May 17, 1996)

It is generally believed that higher order differencing schemes for the convection transport term, e.g., the QUICK scheme and its variants, are superior to the first order simple upwind differencing scheme in the sense that the former produces less numerical diffusion than the latter. In this paper it is shown that this conclusion is no more correct when the flow changes its direction quite rapidly and the grid density is not sufficient. In this situation the simple upwind differencing returns much steeper change of convective variables than higher order schemes. The failure of usual higher order schemes for this flow condition is attributed to the ignorance of convection direction of variables, and a new convection scheme sensitized to the direction of convective transport of a scalar quantity is devised and applied to typical benchmark flows. Results show that the proposed scheme is sufficiently accurate for computation of scalar fields, and also show the optimum behavior for tested problems.

Key Words: Convection Scheme, Simple Upwind Difference Scheme (SUDS), Quadratic Upstream Interpola on for Convective Kinematics (QUICK), Total Variation Diminishing (TVD) Constraint, Convection Direction Constraint (CDC).

1. Introduction

Although many engineering problems now get benefits from the computational fluid dynamics technique, the technique still has problems to be addressed. They stem from two different sources: a mathematical modelling of the flow and a numerical technique employed to solve the model equations. For a simple shear flow where most part of fluid flows along one direction, the mathematical model controls the quality of numerical solutions, while numerical techniques have little effect. But when the flow direction is multi-dimensional, numerical methods employed manifest its performance and solutions are depending on both of the above two aspects. Present study is focused on the latter aspect, specifically on the numerical approximation of convective transport of a fluid mechanical quantity.

Numerical approximation of convective spatial transport, $\partial(u_j\phi)/\partial x_j$, at control surfaces does a key role in predicting accurate heat and fluid flow field. The natural choice of the central difference scheme (CDS, Patankar, 1980) is unacceptable because it forms unstable system matrix. The absolutely stable simple first order upwind scheme (SUDS, Patankar, 1980) has been hardly used because it produces too much unphysical, numerical diffusion, and thereby too broaden profiles for a fluid mechanical quantity. A different strategy formulating the convective and diffusive spatial transport collectively has been pursued by some researchers: The well-known exponential difference scheme of Allen & Southwell (1955) and its variants, e.g. the Hybrid difference scheme of Spalding (1972) and the Power-Law difference scheme (PLDS) of Patankar (1980), have been most popular during the

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last couple of decades because they produce stable matrix structure and smooth profiles of dependent variables. And most commercial CFD codes adopt these schemes as a standard option. However, unfortunately, uncomfortable cases with the exponential-based scheme have been increased when one gradually turns to look flow fields of engineering problem where the topology of geometry is complex and, thereby, the fluid flow is multidimensional. The same mood has often been felt even for a flow with a simple geometry when the flow has a new physical element which has not been considered before. Because of these reasons, Leonard & Drummond (1995) suggested not to use the exponential-based scheme for a predictive purpose. A more accurate convection scheme QUICK (Quadratic Upstream Interpolation for Convective Kinematics) proposed by Leonard (1979) has been attractive because it reduces the numerical diffusion greatly, but its implementation in a CFD code and practical usage have been deferred because it suffers from unphysical oscillation of dependent variables where its spatial gradient is high. This oscillation is undesirable, especially for a turbulent flow, because the estimated face value may take negative value even for a positive definite quantity, for example the turbulent kinetic energy and its dissipation rate, and thereby the computation may blow up during the numerical iteration. As it is demonstrated by Gaskell & Lau (1988), the increase of grid density does not resolve this problem in principle. So a usual practice for a turbulent flow is to use the QUICK scheme for continuity and momentum equations but exponential schemes for turbulence equations assuming that the source/sink terms dominate the spatial transport terms in the turbulence equations (for example, Lien & Leschziner, 1993).

Such situation met a turning point when Harten (1983) and Sweby (1984) proposed a concept of TVD (Total Variation Diminishing) constraint for the convective transport approximation. This constraint acts to preserve monotonic variation of dependent variables and to eliminate unphysical oscillation. Some higher order convection schemes satisfying the TVD constraint have been followed: the SMART (Sharp and Monotonic Algorithm for Realistic Transport) scheme of Gaskell and Lau (1988), the SHARP (Simple High Accuracy Resolution Program) scheme of Leonard (1988), the SOUCUP (Second-Order Upwind-Central differencing- first-order Upwind) scheme of Zhu & Rodi (1991), and the UMIST (Upstream Monotonic Interpolation for Scalar Transport) of Lien & Leschziner (1994) are typical examples. In all these proposals an appropriate switching is done among basic interpolation methods, e.g. SUDS, CDS, QUICK, etc. to achieve the numerical accuracy and the monotonic variation of dependent variables.

In this study it is noted that a scalar quantity has a preferential direction for convective spatial transport, and a new convection scheme sensitized to the direction is proposed. For this scheme the second order upwind scheme of Atias, Wolfshtein, & Israeli (1977) is adopted as a parent one because, according to Shyy (1985), it is most satisfactory in general among SUDS such as skew upwind of Raithby (1976), second order upwind, second order CDS, and QUICK. Also, ULTRA constraint of Leonard (1988) is used to achieve the TVD behavior.

2. A New Proposal

We consider an incompressible, steady, 1-dimensional flow for simplicity of discussion. The transport equation for a fluid mechanical quantity ϕ is written as follows:

$$\frac{d}{dx}(u\phi)=\frac{d}{dx}\left(\Gamma\frac{d\phi}{dx}\right)+S \tag{1}$$

where u, Γ, and S represent velocity, physical diffusivity, and source/sink term, respectively. Integration of Eq. (1) over the 1-dimensional control volume shown in Fig. 1 gives

$$\begin{aligned} u_e\phi_e-u_w\phi_w &= \left(\Gamma\frac{d\phi}{dx}\right)_e-\left(\Gamma\frac{d\phi}{dx}\right)_w+\int_{x_w}^{x_e}Sdx \\ &\approx \frac{\Gamma_e(\phi_E-\phi_P)}{\delta x_e}-\frac{\Gamma_w(\phi_P-\phi_W)}{\delta x_w} \\ &\quad +S\delta x_P \end{aligned} \tag{2}$$

This algebraic equation can now be handled

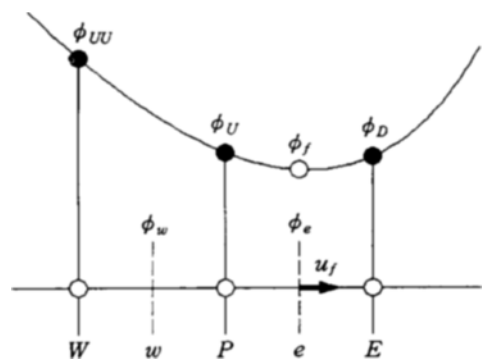

Fig. 1. One-dimensional, stencil for estimation of ϕ_f.

numerically if control volume face values u_e, u_w, ϕ_e, ϕ_w, Γ_e, and Γ_w are approximated properly. The main issue in this equation is how to approximate convection term, or the left hand side of Eq. (2), and it is known as convection scheme. The natural choice is taking a simple algebraic mean of neighboring values, or the CDS. However, unfortunately, this difference scheme leads to unstable matrix structure.

In approximating the control volume face value, one usually starts with the Taylor series expansion. The approximation concept of Leonard's QUICK scheme is shown in Fig. 1. Note that two upstream (ϕ_U and ϕ_{UU}) and one downstream (ϕ_D) values at grid nodes are used to evaluate the value at the control volume face. When $u_f>0$, the control volume face value ϕ_f can be determined from the following three Taylor series expansions:

$$\phi_D = \phi_f + \frac{\Delta x}{2}\phi'_f + \frac{\Delta x^2}{8}\phi''_f + O(\Delta x^3)$$
$$\phi_U = \phi_f - \frac{\Delta x}{2}\phi'_f + \frac{\Delta x^2}{8}\phi''_f - O(\Delta x^3)$$
$$\phi_{UU} = \phi_f - \frac{3\Delta x}{2}\phi'_f + \frac{9\Delta x^2}{8}\phi''_f + O(\Delta x^3) \quad (3)$$

where it is assumed that the grid spacing is uniform. By eliminating the first and second derivatives and neglecting higher order terms, the estimation is

$$\phi_f \approx \frac{3\phi_D + 6\phi_U - \phi_{UU}}{8} = \mathrm{ftn}(\phi_D,\phi_U,\phi_{UU}) \quad (4)$$

In fact all higher order TVD schemes mentioned before use the same argument (ϕ_D,ϕ_U, ϕ_{UU}), and the difference among them is on the selection of the interpolation function. One may use more upstream and/or downstream values to improve the accuracy. It is usually accepted that these estimations offer higher accuracy than the SUDS.

$$\phi_f = \phi_U \quad (5)$$

It should be noted here that the above Taylor series expansions may be not accepted in certain circumstances in a physical sense. Consider a situation where the convection dominates the flow field and the diffusion is absent. In that case, a scalar quantity ϕ is simply convected down with the fluid stream, and it is clear that the value of the scalar quantity at a point is insensitive to the downstream value:

$$\phi_f \neq \mathrm{ftn}(\phi_D) \quad (6a)$$

The same consideration leads to the following constraint:

$$\phi_f \neq \mathrm{ftn}(\phi_{UU}) \text{ if } \mathrm{sign}(u_f)\cdot\mathrm{sign}(u_{UU})<0 \quad (6b)$$

These two constraints, Eqs. (6a) and (6b), are here termed as CDC (Convection Direction Constraint). Note that the QUICK scheme and all higher-order TVD schemes mentioned in Sec. 1 do not satisfy these new constraints, but the SUDS always do. Because of this difference, on the contrary to the usual belief, the SUDS gives much better prediction (or, lower numerical diffusion) in a particular flow configuration than the QUICK scheme as we will see later in Sec. 3. Recognizing this fact a new convection scheme blending the SUDS and second-order upwind difference scheme is proposed below:

$$\phi_f = \mathrm{ftn}\,(\phi_U,\phi_{UU},u_f,u_{UU}) = \phi_U + g(u_f,u_{UU})\frac{\phi_U - \phi_{UU}}{2} \quad (7)$$

Note here that the face value ϕ_f is assumed to depend on upstream velocities as well as upstream scalar values. This equation becomes the SUDS if the switching function g=0, and the second-order upwind difference if g=1. It is understood that the second term of the right hand side represents an anti-diffusive higher order correction to the diffusive SUDS given by the first term. The first constraint, Eq. (6a), is satisfied automatically because downstream values are dropped in the above functional form. The second constraint, Eq. (6b), is satisfied by employing the following transition function permitting smooth change over between two options:

$$g(u_f, u_{UU}) = \sin\left(\frac{\pi}{2}\left\langle\left\langle \frac{u_{UU}}{u_f}, 0\right\rangle_{\max}, 1\right\rangle_{\min}\right) \quad (8)$$

There is no definite reason to use this sine function, and one may devise a different one, for example, a simple on-off function, a power function, etc. Due to the relatively small number of test cases in this study, no particular attention is given for the function. Because the above formulation is not free from unphysical oscillations, a TVD constraint should be employed. In this study, the ULTRA constraint of Leonard & Drummond (1995) is used. The computation step to estimate the face value is summarized below:

Step 1 The higher order estimation (HOE) is obtained by applying the second-order upwind scheme:

$$\phi_f^{HOE} = \frac{3\phi_U - \phi_{UU}}{2} \quad (9)$$

Step 2 The ULTRA constraint is applied to the estimation for the monotonicity:

$$\begin{aligned} \tilde{\phi}_U \le \tilde{\phi}_f^{HOE} \le 1 \quad &\text{if} \quad 0 \le \tilde{\phi}_U \le 1 \\ \tilde{\phi}_f^{HOE} \to 0 \quad &\text{if} \quad \tilde{\phi}_U \to 0_+ \\ \tilde{\phi}_f^{HOE} = \tilde{\phi}_U \quad &\text{if} \quad \tilde{\phi}_U < 0 \text{ or } \tilde{\phi}_U > 1 \end{aligned} \quad (10)$$

where

$$\tilde{\phi} = \frac{\phi - \phi_{UU}}{\phi_D - \phi_{UU}} \quad (11)$$

Step 3 The TVD-corrected estimation is obtained by inversing the normalization:

$$\phi_f^{TVD} = \phi_{UU} + \tilde{\phi}_f^{HOE}(\phi_D - \phi_{UU}) \quad (12)$$

Step 4 The convection direction constraints are applied:

$$\phi_f = \phi_U + g(u_f, u_{UU})(\phi_f^{TVD} - \phi_U) \quad (13)$$

For a stable iterative computation, the so-called deferred-correction technique by Khosla & Rubin (1974) is adopted in the final expression: The second term on the right hand side is lumped into the source term, and only the first term is serving as an apparent convection. The resulting system matrix is the same with that of the SUDS.

At this point one may argue that the CDC is not appropriate for the momentum equation because the fluid momentum at a point is influenced by the downstream condition through the pressure reflection. Clear solution is applying the CDC only for a scalar equation and not for momentum equations. However, usually one favors uniform application of a single convection scheme for all transportable variables. Note that the downstream information is partially transferred to the approximation through the TVD constraints. Anyway the presnt scheme should return better result than the SUDS because the formal truncation error is $\sim O(\Delta x^2)$.

3. Applications

3.1 Pure convection of a step profile in a unidirectional flow

The first test problem is an imaginary pure convection of a temperature T in a prescribed, unidirectional velocity field: the hot and the cold fluid flows are in the same direction, and the flow configuration is shown in Fig. 2(a). This benchmark case has been adopted by Gaskell & Lau (1988) and Shyy (1985) to test the accuracy of convection schemes. The computation coordinate is rotated intentionally by 45 degree to the 1-dimensional flow direction in order to maximize numerical errors associated with the convection scheme, and the convection equation is written as follows:

$$\frac{\partial uT}{\partial x} + \frac{\partial vT}{\partial y} = 0. \quad (14)$$

Because there is no diffusive transport the temperature of a fluid particle does not change as it is convected downwards. So the extremely sharp gradient of temperature invoked at the boundaries is maintained within the flow domain. Numerical solutions with the SUDS, QUICK, ULTRA-QUICK, and the present proposal are obtained by using a collocated-grid version of the TEACH code. Results with a 21x21 regular mesh are presented in Fig. 2(b). An increased grid density

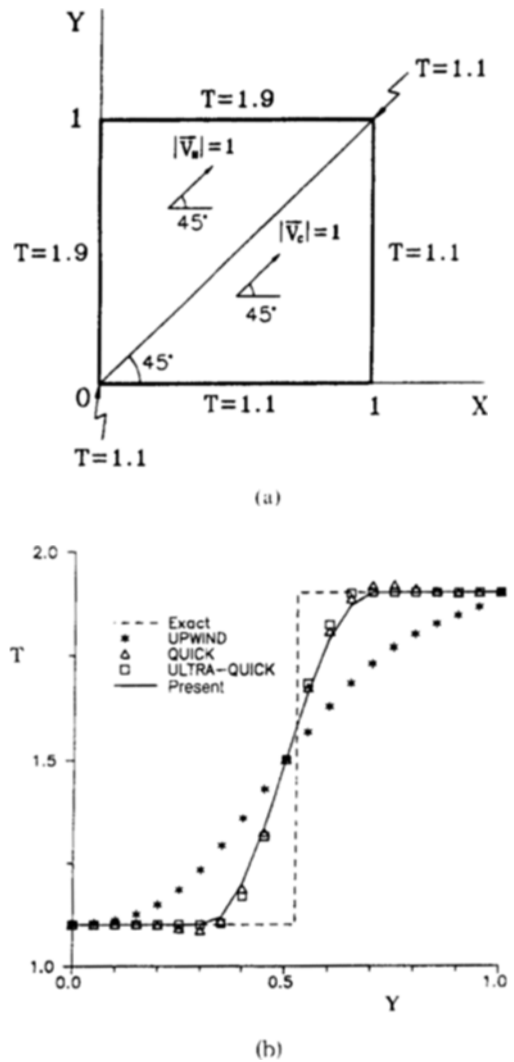

Fig. 2. Pure convection of a step profile in a unidirectional flow configuration (a) and comparisons of the predicted temperature profile (b).

does not affect the general discussion and conclusion which will be followed below.

The first-order accurate SUDS returns a very diffusive temperature profile due to the influence of artificial numerical diffusion. Of course a false-diffusion-free solution can be obtained by aligning one axes of the coordinate with the flow direction for this particular problem, but it is difficult to obtain such grid arrangement in general flow condition. On the other hand, the steep gradient is fairly well predicted by the QUICK scheme. However, unfortunately, the profile shows overshoot within the hot stream, and undershoot within the cold stream, and both peaks lie outside the physical bounds of the solution. The undershoot is more dangerous because it may return a negative value for a positive definite scalar quantity, e.g. the turbulent kinetic energy k and its dissipation rate ε. Because of this reason the QUICK scheme is usually not adopted for turbulence equations. The oscillation free, monotonic variation of temperature is achieved by the ULTRA-QUICK while preserving the sharp changeover of the QUICK. The SMART algorithm of Gaskell & Lau gives comparable numerical accuracy with the ULTRA-QUICK. The result isn't included here for simplicity of presentation. Although the present proposal based on the second-order accurate upwind difference returns slightly slower changeover of temperature profile than the third-order accurate QUICK and its variant ULTRA- QUICK, it is supposed to be comparable for a practical purpose. The present scheme can be upgraded by employing more upstream ϕ values along with an appropriate, extended convection direction constraint (CDC) to yield the third-order or even higher numerical accuracy. However, this job has not been tried here, mainly because the aim of present study is to prove validity of the CDC concept and partly because, for a practical CFD problem, dominance of the third-order accurate scheme over the second-order accurate one is not definite at the moment (Shyy, 1985).

3.2 Pure convection of a step profile in a bidirectional flow

The second test problem is similar to the previous case, but the hot and the cold streams are moving in opposite direction as it is depicted in Fig. 3(a). This benchmark case has not been tested by others and introduced here for the first time. This situation occurs in a stagnation flow such as an impinging jet flow, and in a recirculating flow. Again, the extremely sharp gradient of temperature distribution invoked at the flow boundaries is maintained within the flow domain due to the absence of physical diffusion. Details

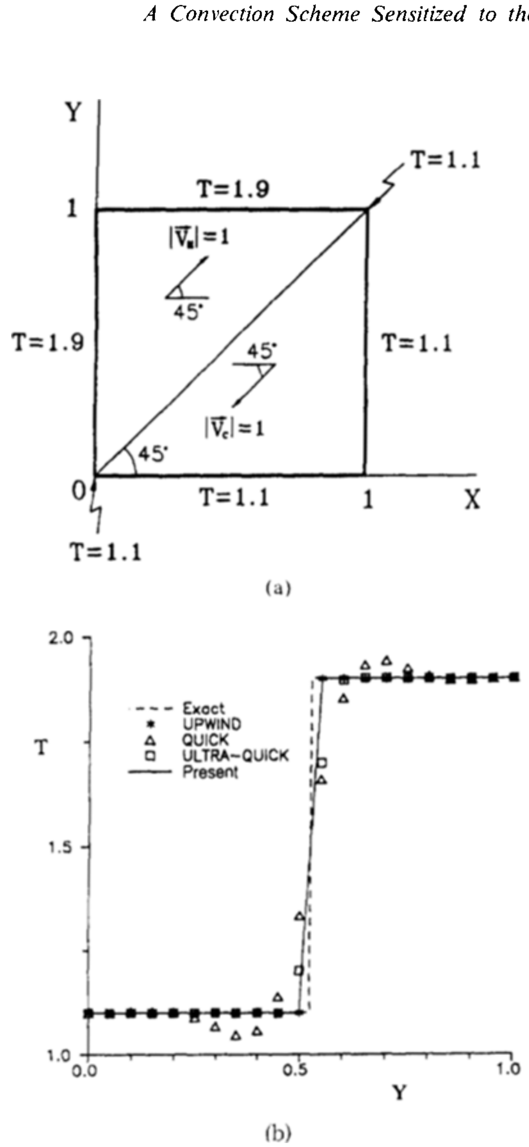

Fig. 3. Pure convection of a step profile in a bidirectional flow configuration (a) and comparisons of the predicted temperature profile (b).

of numerical aspects are the same with the first case.

Within a CFD research community, it is generally believed that the higher order schemes, typically the QUICK and its variants with a TVD limiter, produces less numerical diffusion than the first-order simple upwind scheme. However, as it can be found in Fig. 3(b), for this benchmark case, the SUDS gives much steeper changeover of the temperature profile between the hot and cold stream than the QUICK and ULTRA-QUICK. The reason is as follows: For the SUDS, the information of one fluid stream can not be transferred across the interface between the hot and cold stream flow in the opposit direction because the estimated temperature at a control volume face depends on the pure upstream node value and does not depend on the downstream node value. However, for the QUICK and ULTRA-QUICK, the downstream information is transferred across the interface between the two streams because the estimated temperature at the control surface depends on the value at the downstream point located in a stream flowing in a opposit direction. Again, the QUICK scheme shows unphysical oscillations near the sharp slope. The present proposal sensitized to the convection direction of a scalar produces the sharp temperature transition between two-streams, and performs much better than other higher order schemes.

3.3 Laminar natural convection in a tall cavity

As it has been shown by Leonard & Drummond (1995), the buoyancy-driven laminar flow in a two-dimensional rectangular cavity (see Fig. 4(a)) is a good benchmark problem to test the accuracy of convection schemes. The flow near the hot-wall rises along the wall, turns at the top of the cavity, and then falls along the cold-wall as it looses heat. Whereas the flow near the mid-plane between the two vertical walls forms multiple 2-dimensional rotating cells for a certain flow condition as reported by Vest & Arpaci (1969). Leonard & Drummond (1995) have showed that these characteristic cells do not appear if the convection scheme produces too much numerical diffusion. Applying the Boussinesq approximation, the flow equation can be non-dimensionalized to yield:

$$G_R\left(\frac{\partial u\omega}{\partial x}+\frac{\partial v\omega}{\partial y}\right)=\left(\frac{\partial^2\omega}{\partial x^2}+\frac{\partial^2\omega}{\partial y^2}\right)+\frac{\partial T}{\partial x} \quad (15)$$

$$G_R\left(\frac{\partial uT}{\partial x}+\frac{\partial vT}{\partial y}\right)=\frac{1}{P_R}\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}\right) \quad (16)$$

$$\frac{\partial^2\Psi}{\partial x^2}+\frac{\partial^2\Psi}{\partial y^2}=-w \quad (17)$$

where the vorticity ω and stream function Ψ are defined by

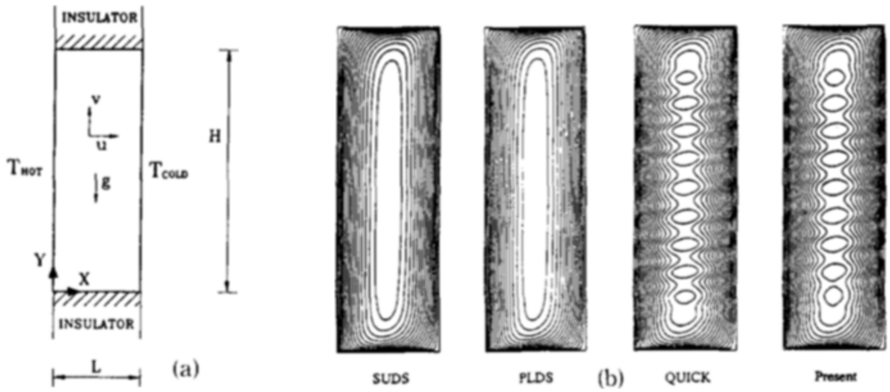

Fig. 4. The tall cavity configuration (a) and predicted streamline patterns (b).

$$\omega=\frac{\partial v}{\partial x}-\frac{\partial u}{\partial x} \tag{18}$$

$$u=\frac{\partial \Psi}{\partial y},\ v=-\frac{\partial \Psi}{\partial x} \tag{19}$$

Here the pressure is eliminated from flow equations by adopting the $\omega-\Psi$ formulation. The Grashsof number G_R and the Prandtl number P_R are defined by

$$G_R=\frac{\beta g L^3 \Delta T}{\nu^2} \text{ and } P_R=\frac{\nu}{\alpha} \tag{20}$$

In the above relations, β,ν,α,g,L and ΔT are the thermal expansion ratio, the kinematic viscosity, the thermal diffusivity, the gravitational accelerllation, the width of cavity, and the temperature difference between hot and cold walls, respectively. The height of enclosure $H=33$, $G_R=9500$, and $P_R=0.71$ for present computation. Boundary conditions are as follows:

$$\begin{aligned}
&u=\frac{\partial \Psi}{\partial y}=0 && \text{at } y=0 \text{ and } y=H\\
&v=-\frac{\partial \Psi}{\partial x}=0 && \text{at } y=0 \text{ and } y=H\\
&\Psi=0 && \text{at } x=0,\ x=1,\ y=0 \text{ and } y=H\\
&T=1 && \text{at } x=0\\
&T=0 && \text{at } x=0\\
&\frac{\partial T}{\partial y}=0 && \text{at } y=0 \text{ and } y=H
\end{aligned} \tag{21}$$

The numerical solver is the same with previous two cases. A 31x129 grid having uniform spacing in the x- and y-directions is used.

Figure 4(b) shows computed streamline patterns with various convection schemes, and confirms the finding of Leonard and Drummond (1969) : the SUDS and PLDS do not show any secondary rotating cells, and the third order accurate QUICK scheme forms the characteristic cells. The present scheme formally second order accurate also produces very similar secondary rotating cells: the number and spacing of rotating cells are the same. A slight difference between the QUICK and present scheme is observed in the shape of rotating cells formed near top and bottom insulation walls. However, unfortunately, it is difficult to compare the relative performance of two schemes because experimental results are not available. Note that the CDC is used for all transport equations uniformly. This result confirms that the present scheme produces more reliable result than the usual SUDS or PLDS for a practical problem, especially when experimental data are absent. And it is supposed that the present one provides nearly the same prediction accuracy with the QUICK and its variants for a practical purpose.

4. Concluding Remarks

In this study, it has been shown that the higher order QUICK scheme and various TVD schemes are not always superior to the simple upwind difference scheme, and, in fact, that the converse is true in some flow conditions. The problem has occurred due to the negligence of convective character of a scalar quantity. The present paper has noted that a scalar quantity is simply convected down with a fluid particle if there is no diffusive transport, and the CDC (Convection Direction Constraint) concept has been introduced for a scalar quantity. A new numerical model for convective transport for the scalar satisfying both the TVD constraint and CDC has been devised, and applied to typical benchmark flows. The numerical result shows that the present scheme mimics the convective transport of a scalar quantity quite well. In predicting the convective scalar field, owing to the CDC, the present scheme performs better than the QUICK and ULTRA-QUICK if the flow direction changes rapidly. It should be admitted that the CDC concept is not correct, in a strict physical sense, for a numerical modelling of the convective mometum transport because the mometum field has an ellitic nature and the downstream information may be feedback to upstream through the pressure reflection. However, the third test case shows that, for a practical purpose, it can be used with sufficient numerical accuracy and without unrealistic physical behavior. In fact, downstream information is transfered backward through the TVD constraint partially. A recirculating zone and a stagnation region are common for an engineering CFD problem and they form the aforementioned flow situation. If there is a significant variation of a scalar, it is expected that the present proposal would provide better prediction. In fact, preliminary numerical study of heat transfer of impinging jet flows by the author showed a sensible change of the stagnation point Nusselt number depending on the numerical model for the convective transport. These results are in due course to be appeared.

Acknowledgements

Reviewer's comments were valuable for completeness of this paper.

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