Comparative Evaluation of Convection Schemes for the Numerical Analysis of Thermal Stratification in a Horizontal Circular Pipe

Yun Il Kim, Sang Jin Cho, Wee Kyung Kim, and Jong Chull Jo
Korea Institute of Nuclear Safety
19 Kusung-dong, Yusung-ku, Taejon 305-338, Korea

Abstract

This paper presents a comparative evaluation of four convection schemes, QUICK, HLPA, HYBRID and COPLA for the numerical analysis of unsteady stratified flow and conjugate heat transfer in a circular pipe. All the schemes are formulated on a non-uniform, non-orthogonal grid so that they can be applicable to the practical engineering flow calculations. The relative performances among the four schemes are investigated by applying them to the numerical analysis of thermal stratification in a pressurizer surge line of pressurized water reactor (PWR) plant. It is seen from the calculation results that all the bounded schemes might be applicable for the solutions of thermal stratification problem in a horizontal circular pipe, the HLPA and COPLA schemes results in nearly the same solution and are more superior both in accuracy and convergence to the QUICK and HYBRID schemes.

1. Introduction

Development of an efficient convection scheme which is simple to implement but is free of false diffusion has been one of the major tasks for the computational fluid dynamicists over the last two decades. The classical lower-order schemes such as the upwind scheme, the hybrid central/upwind scheme and the power-law scheme[1] are unconditionally bounded and highly stable but highly diffusive when the flow direction is skewed relative to the grid lines. A simple remedy to overcome the false diffusion is to use a fine enough grid. However, such a practice is not practical due to the requirement of excessive computer storage and computational efforts, especially in the complex three-dimensional flow calculations.

Considerable efforts have been made toward the development of the improved differencing schemes, mainly in two directions. One is raising the order of the scheme and the other is taking into account the multidimensional nature of flow. The QUICK(Quadratic Upstream Interpolation for Convective Kinematics) scheme[2] and the second-order upwind scheme[3] belong to the former approach and the skew-upwind scheme[4] the latter. These schemes have been successful in increasing the accuracy of the solution, but all suffer from the boundedness problem, resulting in an oscillatory solution behavior in regions of steep gradient which can lead to the numerical instability.

Recently Gaskell and Lau[5] developed a higher-order bounded scheme named SMART(Sharp and Monotonic Algorithm for Realistic Transport) employing a composite approach in which the high resolution schemes are combined with the lower-order bounded schemes. Leonard[6] also proposed a similar bounded scheme of third-order accuracy named SHARP(Simple High-Accuracy Resolution Program). These two schemes have resolved the aforementioned boundedness problem without much deteriorating the accuracy of the higher-order scheme. However, numerical experiments[7] have shown that these schemes need an under-relaxation treatment at each of the control volume cell faces in order to overcome the oscillatory convergence behaviors. This deficiency leads to the increase of the computer storage requirement, which may pose a practical constraint to their use in the complex three-dimensional turbulent flow calculations.

Subsequent studies by Zhu and Rodi[8], Zhu[9], Shin and Choi[10] and Choi et al[11] have proposed bounded convection schemes which are free of oscillatory convergence behaviors by choosing simple characteristics in the normalized variable diagram, such as piecewise-linear profile (SOUCUP : Second-Order
Upwind-Central differencing-first-order UPwind), a parabolic profile(HLPA: Hybrid Linear/Parabolic Approximation), a cubic profile (SMARTER: SMART Efficiently Revised) and a combination of piecewise linear profiles (COPLA: Combination Piecewise Liner Approximation). These schemes are very simple to implement and computationally cost effective. Recently, Choi and Lee[12] have evaluated some Higher-order bounded convection schemes the numerical solutions of the pure convection of a scalar variable problem and the laminar low in lid-driven cavity.

This study aims to perform the comparative evaluation of above four convection schemes, QUICK, HLPA HYBRID and COPLA, in the thermally stratified flow calculations under highly convective conditions. All the schemes are formulated on a non-uniform, non-orthogonal grid so that they can be applicable to the practical engineering flow calculations. The relative performances among the schemes are investigated by applying them to the numerical analyses of thermal stratification in a pressurizer surge line of pressurized water reactor(PWR) plant.

2. Mathematical Formulation

2.1 Governing Equations

To evaluate the applicability of four convection schemes considered herein to the numerical analysis of thermally stratified flow in a horizontal circular pipe, the thermal stratification in a pressurizer surge line of PWR plant [13-15] is chosen as a test problem in this study.

For this purpose, consider the same situation as in the work by Jo et al.[14], where hot fluid and cold fluid in the laminar low in lid-driven cavity.

\[
\frac{\partial}{\partial t} U_1 + \frac{\partial}{\partial x} U_2 = 0
\]

(1)

\[
\frac{\partial}{\partial t} (J, u_i) + \frac{\partial}{\partial x} \left[ U_i u_i - \frac{1}{Re} J \left( \frac{\partial u_i}{\partial x} D_{ij} + \frac{\partial u_j}{\partial x} D_{ij} + b_i \frac{1}{Re} \right) + \frac{1}{PrRe} T \right] = \frac{Gr}{Re} \left[ \frac{\partial T}{\partial x} D_{ij} \right]
\]

(2)

\[
\frac{\partial}{\partial t} (J, u_i) + \frac{\partial}{\partial x} \left[ U_i u_i - \frac{1}{Re} J \left( \frac{\partial u_i}{\partial x} D_{ij} + \frac{\partial u_j}{\partial x} D_{ij} + b_i \frac{1}{Re} \right) + \frac{1}{PrRe} T \right] = 0
\]

(3)

\[
\frac{\partial}{\partial t} (J, u_i) + \frac{\partial}{\partial x} \left[ U_i u_i - \frac{1}{Re} J \left( \frac{\partial u_i}{\partial x} D_{ij} + \frac{\partial u_j}{\partial x} D_{ij} + b_i \frac{1}{Re} \right) + \frac{1}{PrRe} T \right] = 0
\]

(4)

where

\[
U_1 = (u_1 b_1^1 + u_2 b_2^1), \quad U_2 = (u_1 b_1^2 + u_2 b_2^2), \quad D_{ij} = b_i b_j^T, \quad w_i = \frac{\partial u_i}{\partial x}
\]

(5)

and the geometric coefficients \( b_i^T \) represent the cofactors of \( \frac{\partial y_i}{\partial x_j} \) in the Jacobian matrix of the coordinate transformation \( y_i = y(x_i) \), and \( J \) is the determinant of the Jacobian matrix. In the above equations (1) - (4), \( \rho \), \( \mu \), \( k \), \( c_p \), \( \beta \) and \( g \) denote respectively density, dynamic viscosity, pressure, thermal conductivity, the specific heat, volumetric coefficient of thermal expansion, and the gravitational acceleration. In addition, \( u_i \) are the Cartesian velocity components in the \( y_i \) direction. \( W_0 \) is a specified constant bulk velocity of
stratified fluid in the $x^3$ direction, and $r_i$ is the inner radius of the pipe.

2.2 Initial and Boundary Conditions

As mentioned previously, the pipe wall is initially at the temperature of cold fluid $T_c$, and is suddenly exposed to hot fluid at $T_h$. The initial conditions for this are given as

\[
\begin{align*}
  u_i &= 0 \quad (i = 1, 2) \text{ in the whole solution domain, } t = 0 \quad (6a) \\
  T &= 0 \text{ in the pipe wall and the cold fluid layer, } t = 0 \quad (6b) \\
  T &= 1 \text{ in the hot fluid layer, } t = 0 \quad (6c)
\end{align*}
\]

Because the solution domain is symmetrical thermally and geometrically, only half of the region is needed to analyze. Thus along the symmetry line, the symmetry boundary conditions is applied for both velocity and temperature. On the solid wall, the velocity of the fluids vanishes. For this situation the boundary conditions are given by

\[
\begin{align*}
  u_i &= 0 \quad (i = 1, 2) \text{ at the inner surface of the pipe, } t > 0 \\
  \frac{\partial T}{\partial n} &= -\frac{B_i(T - T_c)}{a} \text{ at the outer surface of the pipe, } t > 0 \\
  \text{where} \quad a &= (r_o - r_i)/r_i \quad \text{and} \quad B_i = h(r_o - r_i)/k_i \\
  u_z &= 0, \quad \frac{\partial u_i}{\partial x^3} = 0, \quad \frac{\partial T}{\partial x^3} = 0 \text{ at the symmetry plane, } t > 0
\end{align*}
\]

where $n$ is the outward normal to the surface of the wall, $T_w$ is the temperature of environment outside the pipe, $h$ is heat transfer coefficient, $k_i$ is the thermal conductivity of the pipe material, and $r_o$ is the outer radius of the pipe.

2.3 Solution Domain Discretization

The governing equations (1) – (4) are solved numerically by a finite volume approach, requiring the discretization of the solution domain into a finite number of quadrilateral control volume cell whose faces are coincided with the non-orthogonal curvilinear coordinate lines.

A typical discretized domain is presented in Fig. 2, and also a typical control volume cell is shown in Fig. 3. The values of all computed variables are stored at the geometric center of each control volume cell. The interface between the hot and cold fluids is arranged here to align with a boundary between two rows of cells, i.e. a gridline.

To obtain the curvilinear non-orthogonal mesh shown in Fig. 2, it is assumed that the solution domain is the cross-section of a pair of eccentric cylinders as shown in Fig. 4. The center of the inner solid cylinder is coincided with the intersecting point of the fluid interface and the vertical symmetry line passing the center of the pipe.

The outer cylinder is the pipe subjected to internally stratified flow, and the inner cylinder has such a small size of diameter that the effect of its presence on the calculations can be negligible. Thus, the following boundary conditions are applied to the outer surface of the inner solid cylinder with such an infinitesimal diameter.

\[
\begin{align*}
  \frac{\partial u_i}{\partial x^3} &= 0, \quad \frac{\partial T}{\partial x^3} = 0 \quad (i = 1, 2) \text{ at the outer surface of the infinitesimal inner cylinder, } t > 0
\end{align*}
\]

Dislocating the inner solid cylinder either downward or upward can easily control the level of the fluid interface with a horizontal straight-line configuration. The grid is generated by using an algebraic method. In this study, the calculations are performed with a grid of 77×62, forming 76 divisions in the circumferential direction and 61 divisions in the radial direction.

2.4 Momentum Interpolation Method

For a better resolution of flow field in complex geometries, recently several investigators have developed various calculation methods of momentum equations employing the non-orthogonal, body-fitted coordinates. Among these methods, the non-staggered, momentum interpolation method originally developed by Rhie and
Chow [16] is known to be one of the efficient methods and has been widely used because of its simplicity feature of algorithm. In this method, the momentum equations are solved at the cell centered locations using the Cartesian velocity components as dependent variables and the cell face velocities are obtained through the interpolation of the momentum equations for the neighboring cell centered Cartesian velocity components. In the present analysis, the modified version of the Rhie and Chow’s scheme [15] is used to obtain a converged solution of unsteady flow that is independent of the size of time step.

2.5 Discretization of Transport Equations

In the finite volume approach, the transport equations, Eqs. (1)-(4), are integrated over a control volume shown in Fig. 3. The resulting equation of a general dependent variable $\phi$ can be written as follows

$$
\left( a_p - a_{p-1} \right) \frac{\Delta V}{\Delta t} + F_e - F_w + F_n - F_s + S_\phi \Delta V + S^b_\phi = 0
$$

(9)

where $a_p$ and $a_{p-1}$ denote, respectively, the new and previous values of variable at the nodal point $p$. $\Delta V$ and $\Delta t$ mean the control volume and the time step, respectively. $F$ represents the total flux of $\phi$ across the cell face and $S^b_\phi$ is the sum of the non-orthogonal diffusion terms. The total flux at the west face, for example, can be written as follows with the diffusion term approximated by the central differencing scheme.

$$
F_w = C_w \phi_w - D_w (\phi_p - \phi_w)
$$

(10)

where

$$
C_w = (\rho U)_w, \quad D_w = \frac{1}{2} \left( \frac{1}{2} \right)
$$

(11)

The evaluation of $\phi_p$ plays a key role in determining the accuracy and the stability of numerical solutions. For example, the $\phi_p$ is evaluated as follows when one uses the first-order upwind scheme

$$
\phi_p = U^+_w \phi_w + U^-_w \phi_p
$$

(12)

where $U^+_w$ and $U^-_w$ are the indicators of the local velocity direction such that

$$
U^+_w = 0.5(1 + \sqrt{U'_w / U''_w}),
$$

$$
U^-_w = 1 - U^+_w (U'_w \neq 0)
$$

(13)

Incorporation of Eq. (10) and Eq. (12) and similar expressions for the other cell faces leads to following general difference equation

$$
A_p \dot{\phi}_p = A_w \phi_w + A_n \phi_n + A_s \phi_s + b_b
$$

(14)

where

$$
A_w = D_w + C_w U^+_w
$$

$$
A_e = D_e - C_e U^-_e
$$

$$
A_s = D_s + C_s V^+_s
$$

$$
A_n = D_n - C_n V^-_n
$$

$$
A_p = A_e + A_s + A_n + A_s - S^b_\phi \Delta V
$$

$$
b_b = S^b_\phi \Delta V + S^b_\phi
$$

(15)

and $S^C_\phi$, $S^L_\phi$ are the linearized source terms.

The details of implementation of the higher-order bounded schemes will be outlined in the following chapter.

The current high-order bounded schemes are based on the variable normalization by Leonard[6] and the convection boundedness criterion by Gaskell and Lau[5]. Consider, without loss of generality, the west face of control volume. We introduce a normalized variable such that

\[
\hat{\phi} = \frac{\phi - \phi_U}{\phi_D - \phi_U}
\]  

where the subscripts U and D denote the upstream and the downstream locations.

Eq. (16) can be rewritten in terms of nodal point values

\[
\hat{\phi} = \frac{\phi_W - \phi_U}{\phi_D - \phi_W} U_w^+ + \frac{\phi_E - \phi_U}{\phi_W - \phi_E} U_w^-
\]  

Using the above upwind biased normalized variable, the following four schemes can be written as follows:

Central difference scheme

\[
\hat{\phi}_w = (1 - C_2) \hat{\phi}_W + C_2 U_w^+ + [C_2 \hat{\phi}_P + (1 - C_2) Y_w^-]
\]  

First-order upwind scheme

\[
\hat{\phi}_w = \hat{\phi}_W U_w^+ + \hat{\phi}_P U_w^-
\]  

Second-order upwind scheme

\[
\hat{\phi}_w = (1 - C_1) \hat{\phi}_W U_w^+ + (1 - C_1) \hat{\phi}_P U_w^-
\]  

QUICK scheme

\[
\hat{\phi}_w = \left[ (1 + C_1)(1 - C_2) \hat{\phi}_W + C_2 \left( 1 - \frac{C_1(1 - C_2)}{C_1 + C_2} \right) U_w^+ + \left[ C_2 \left( 1 + C_1 \right) \hat{\phi}_P + (1 - C_2) \left( 1 - \frac{C_2 C_3}{1 - C_2 + C_3} \right) U_w^- \right] \right]
\]  

where

\[
C_1 = \frac{\Delta X_w}{\Delta X_w + \Delta X_E}, \quad C_2 = \frac{\Delta X_w}{\Delta X_w + \Delta X_P}, \quad C_3 = \frac{\Delta X_w}{\Delta X_P + \Delta X_E}
\]  

are the geometric interpolation factors defined in terms of the size of control volume cell. For example, is the size of control volume around the calculation point P and is defined as

\[
\Delta X_P = w F + \overline{F}
\]  

The normalized diagrams for these well-known schemes (\(U_w^+ > 0\)) are shown in Fig. 5.

Gaskell and Lau[5] formulated following convection boundedness criterion. Define a continuous increasing function or union of piecewise continuous increasing function F relating the modeled normalized face value \(\hat{\phi}_w\) to the normalized upstream nodal value \(\hat{\phi}_U\) (\(U_w^+ > 0\)), that is \(\hat{\phi}_w = F(\hat{\phi}_U)\). Then a finite difference approximation to \(\hat{\phi}_w\) is bounded if

(i) for \(0 \leq \hat{\phi}_w \leq 1\), F is bounded below by the function \(\hat{\phi}_w = \hat{\phi}_U\) and above by unity and passes through the points (0,0) and (1,1);

(ii) for \(\hat{\phi}_w < 0, \hat{\phi}_w > 1\), F is equal to \(\hat{\phi}_w\).

The convection boundedness criterion is a necessary and sufficient condition for achieving computed boundedness if only three neighboring upstream nodal values are used to approximate representation of the
convection boundedness criterion is shown in Fig. 6.

According to Leonard[6], for any (in general non-linear) characteristics in the normalized variable diagram (Fig. 5),
(i) passing through Q is necessary and sufficient for second-order accuracy
(ii) passing through Q with a slope of 0.75 (for a uniform grid) is necessary and sufficient for third-order accuracy.

The horizontal and vertical coordinates of point Q in the normalized variable diagram and the scope of the characteristics at the point Q for preserving the third order accuracy for a non-uniform grid can be obtained by a simple algebra using Eqs. (18)-(21).

\[
X_Q = \frac{C_2}{C_1 + C_2} U^+ + \frac{1-C_2}{1-C_2 + C_1} U^-
\]
\[
Y_Q = \frac{C_2 (1+C_1)}{C_1 + C_2} U^+ + \frac{(1-C_2)(1+C_1)}{1-C_2 + C_1} U^-
\]
\[
S_Q = (1+C_1)(1-C_2)U^+ + C_2(1+C_1)U^-
\]  

For a uniform grid, \( X_Q = 0.5 \), \( Y_Q = 0.75 \) and \( S_Q = 0.75 \) Following the above criteria by Gaskell and Lau[5] and by Leonard[6], one may choose several bounded characteristics in the normalized variable diagram whose order of accuracy is determined by the shape of the characteristics. Following are four simple possibilities which ensure the second or third-order accuracy.

**The HLPA scheme**

In this scheme, the normalized face value is approximated by a combination of linear and parabolic characteristics passing through the point, O, Q and P in the normalized variable diagram

\[
\hat{\phi}_n = a_n \hat{\phi}_O + b_n \hat{\phi}_C + c_n \hat{\phi}_P^n \quad 0 \leq \hat{\phi}_C \leq 1
\]
\[
= \hat{\phi}_C \quad \text{otherwise}
\]  

where
\[
a_n = 0
\]
\[
b_n = (Y_Q - X_Q^n)/(X_Q - X_Q^n)
\]
\[
c_n = (X_Q - Y_Q)/(X_Q - X_Q^n)
\]  

Zhu[9] developed this scheme on the assumption of uniform grid (in this case), \( a_n = 0, b_n = 0, c_n = -1 \). The original scheme is further extended for use on the non-uniform grid in the present study. This scheme is second-order accurate.

**The COPLA scheme**

Another possible way of devising a third-order accurate scheme is to employ a composite of piecewise linear characteristics in which the QUICK scheme is employed in a range of \( 0.5X_Q \leq \hat{\phi}_C \leq 1.5X_Q \). This scheme is similar to the SMART scheme[5], but is free of convergence oscillation. Such a scheme was proposed by Choi et al[11] employing following characteristics in the normalized variable

\[
\hat{\phi}_n = a_n \hat{\phi}_O + b_n \hat{\phi}_C \quad 0 \leq \hat{\phi}_C \leq 0.5X_Q
\]
\[
=c_n + d_n \hat{\phi}_C \quad 0.5X_Q \leq \hat{\phi}_C \leq 1.5X_Q
\]
\[
=e_n + f_n \hat{\phi}_C \quad 1.5X_Q \leq \hat{\phi}_C \leq 1
\]
\[
= \hat{\phi}_C \quad \text{otherwise}
\]  

where
The normalized variable diagrams for the higher-other bounded schemes considered in the present study are given in Fig. 7.

It is worthwhile mentioning here that the present bounded schemes are very similar to the shock capturing schemes based on the Total Variational Diminishing flux limiters (TVD), which are widely used in the compressible flow calculations. The SOUCUP scheme is similar to the MINMOD (MINimum MODulus) scheme of Roe [17] and the HLPA scheme is similar to the CLAM (Curved Line Advection Method) scheme of Van Leer [18]. The implementation of the higher-order bounded schemes is quite simple. We note that the aforementioned four bounded schemes employ very similar forms of characteristics in the normalized variable diagram. They differ only in the order of the characteristics and the values of the constants. Therefore, it suffices to present the implementation of one scheme here, for example, the HLPA scheme. In the present work, the higher-order schemes are implemented in a deferred correction way proposed by Khosla and Rubin [19].

Eq. (25) can be expressed in terms of the unnormalized variable

\[
\phi_u = \left[ \phi_w + (\phi_p - \phi_{ww}) \left[ a^+ + (b^- - 1) \left( \phi_w - \phi_{ww} \right) \left( \phi_p - \phi_{ww} \right)^2 + c^+ \left( \phi_w - \phi_{ww} \right) \right] \right] U_w^+ + \left[ \phi_p + (\phi_w - \phi_E) \left[ a^- + (b^- - 1) \left( \phi_p - \phi_E \right) \left( \phi_w - \phi_E \right)^2 + c^- \left( \phi_p - \phi_E \right) \right] \right] U_w^-
\]

(29)

Given the switch factors

- for \( U_w > 0 \): \( a^+ = 1 \) if \( \left| \phi_w - 2\phi_p + \phi_{ww} \right| < \left| \phi_w - \phi_E \right| \)
- otherwise \( a^+ = 0 \)

(30)

- for \( U_w < 0 \): \( a^- = 1 \) if \( \left| \phi_w - 2\phi_p + \phi_E \right| < \left| \phi_w - \phi_E \right| \)
- otherwise \( a^- = 0 \)

(31)

the unnormalized form of Eq. (29) can be rewritten as

\[
\phi_u = U_w^+ \phi_w + U_w^- \phi_p + \Delta \phi_u
\]

(32)

where

\[
\Delta \phi_u = U_w^+ a^+ (\phi_p - \phi_{ww}) \left[ a^+ + (b^- - 1) \left( \phi_w - \phi_{ww} \right) \left( \phi_p - \phi_{ww} \right)^2 + c^+ \left( \phi_w - \phi_{ww} \right) \right] + U_w^- a^- (\phi_w - \phi_E) \left[ a^- + (b^- - 1) \left( \phi_p - \phi_E \right) \left( \phi_w - \phi_E \right)^2 + c^- \left( \phi_p - \phi_E \right) \right]
\]

(33)

After the evaluation of the additional term, the implementation of this scheme is the same as that of the first-order upwind scheme. In the SOUCUP and LAPP schemes, the constants are switched according to the value of \( \hat{\phi} \) at the same cell face and for the same flow direction.

4. Application to the Test Problem

All the higher-order bounded schemes described in the previous chapter are implemented in a computer code designed to solve the unsteady conjugate heat transfer and stratified flow in a horizontal curved pipe. The
5. Conclusion

To evaluate the applicability of four convection schemes, QUICK, HLPA, HYBRID and COPLA to the numerical analysis of thermal stratification problem in a horizontal circular pipe, in this study the thermal stratification in a pressurizer surge line of PWR plant is chosen as a test problem and the relative performances among the four schemes are investigated. The following important conclusions can be drawn from the present analysis.

- All the bounded schemes might be acceptable for the applications to the solutions of thermal stratification problem in a horizontal circular pipe.
- QUICK scheme exhibits relatively high and oscillatory value in the top position at the early stage
HYBRID scheme results in relatively more diffusive profiles than the other three convection schemes in the top and bottom positions.

The HLPA and COPLA schemes results in nearly the same solution and are more superior both in accuracy and convergence to the QUICK and HYBRID schemes.

References

Fig. 1 Thermally stratified flow in a circular pipe.

Fig. 2 The curvilinear non-orthogonal mesh.

Fig. 3 A typical control volume cell in the computing mesh.

Fig. 4 The imaginary eccentric cylinder for mesh generation.
Fig. 5 The normalized variable diagram for various well-known schemes.

(Figures not shown in text)

Fig. 6 Diagrammatic representation of the convection boundedness criterion.

Legend
- - - - UPWIND
______ QUICK
_____ SOUCUP
___ HLPA
------ SMARTER
__ LPPA

Fig. 7 The normalized variable diagram for bounded schemes.
Fig. 8 Transient top to bottom wall temperature distributions. (a) on the inner wall (b) on the outer wall
Fig. 9 The variation of the local Nusselt number (Nu).
Fig. 10 Transient isotherms for the four convection schemes (COPLA, HLPA, HYBRID, QUICK)
Fig. 11 Transient maximum wall temperature differences both on the inner and outer wall surfaces.