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Use of Momentum Interpolation Method and Evaluation of Higher-Order Bounded Convection Schemes for Oscillatory Natural Convection of Liquid Metal

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A study on the use of momentum interpolation method and higher-order bounded convection schemes for simulation of oscillatory natural convection of liquid metal in a square cavity is presented. The original Rhie and Chow scheme is modified for unsteady flows to obtain the converged solutions which are independent of the time step size. Two higher-order bounded convection schemes, SOUCUP and COPLA are evaluated, together with HYBRID and QUICK, to test their capability for predicting the oscillatory natural convection. The calculations are performed for $G_r=10^7$, Pr=0.005 employing 42×42 and 82×82 nonuniform grids. The COPLA and QUICK schemes have shown the capability of predicting the oscillatory motion while the HYBRID and SOUCUP schemes have not.

Key Words : Momentum Interpolation Method, Higher-Order Bounded Convection Schemes, Oscillatory Natural Convection, Liquid Metal.

Nomenclature

A	: Coefficient in the discretization equation
b	: Source term in the discretization equation
C_p	: Specific heat
D_u, D_v	: Coefficients of pressure terms
f_e^+	: Geometric interpolation factor
g	: Gravitational acceleration
Gr	: Grashof number
k	: Conductivity
L	: Length of the cavity
Nu	: Nusselt number
P	: Pressure
Pr	: Prandtl number
S_p, S_c	: Linearized source term
T	: Temperature
t	: Time
u_i	: Cartesian velocity components
x_i	: Cartesian coordinate system

Greek symbols

α	: Thermal diffusivity
α_u, α_v	: Relaxation factors
β	: Volumetric coefficient of thermal expansion
Δt	: Time step
ΔV	: Volume
ϕ	: Variable
θ	: Dimensionless temperature
μ	: Viscosity
ν	: Kinematic viscosity
ρ	: Density

Superscripts

$l-1$	: Previous iteration level
$n-1$	: Previous time step
u, v	: Pertaining to u, v velocity components

Subscripts

C	: Pertaining to cold
e, w, n, s	: East, west, north, south faces of control volume
E, W, N, S	: East, west, north, south neighbors of grid point P
H	: Pertaining to hot
nb	: Pertaining to neighboring point

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P : Pertaining to grid point P.
u, v : Pertaining to u, v velocity components

1. Introduction

Natural convection of liquid metal has become an important topic due to its applications in material processing, semiconductor crystal growth and decay heat removal in a liquid metal reactor. An understanding of the natural convection in a liquid metal reactor is very important in securing the structural integrity of the reactor.

The natural convection of liquid metal has not been well understood. The flow is highly nonlinear, and the shape of streamlines is nearly circular. Numerical false diffusion occurs when the flow is oblique to the rectangular shape grid lines. Low-Prandtl-number fluids have a tendency to oscillate at relatively low Rayleigh numbers. Some of the numerical issues associated with the prediction of oscillatory natural convection are the treatment of an unsteady term, the choice of a convection scheme to avoid the numerical false diffusion, and the use of momentum interpolation method for unsteady flows involving large body forces. Cless and Prescott (1996) have studied the treatment of an unsteady term. They have tested the implicit and semi-implicit schemes in advancing the solution in a time domain. The present study deals with the remaining two issues.

Most of previous works used the finite element method (Gresho and Upson, 1983), the stream function-vorticity formulation (Kamakura and Ozoe, 1996), and the staggered grid based the finite volume method (Mohamad and Viskanta, 1991) for the simulation of oscillatory natural convection of liquid metal. The nonstaggered, momentum interpolation method of Rhie and Chow (1983) is used in the present study. After Rhie and Chow proposed a scheme based on the momentum interpolation method, it has been widely used due to its simplicity of algorithm, especially when the numerical grids were nonorthogonal. However, the original Rhie and Chow scheme did not take into account the presence of underrelaxation factors in the discretized momentum equations. Majumdar (1988) found that the converged solution was relaxation factor-dependent and proposed a remedy for this problem. In the present study we propose that a further modification of the Rhie and Chow scheme is necessary for the simulation of unsteady flows to obtain the converged solution which is independent of the time step size.

Mohamad and Viskanta (1989) evaluated four different convection schemes for natural convection of low Prandtl number fluids. They concluded that the first order schemes ware incapable of predicting the oscillatory convection and recommended the central difference scheme for transient simulation. Subsequent study of Mohamad and Viskanta (1991) and Cless and Prescott (1996) also used the central difference scheme for the transient natural convection of low Prandtl number fluids. However, the central difference scheme is unstable when the grid Peclet number is high and is not well used in the general purpose code. Mohamad and Viskanta (1989) used this scheme in the transient calculations using a very small time step.

The higher-order schemes such as the central difference scheme, the QUICK scheme (Leonard, 1979), the second-order upwind scheme (Shyy, 1985) and the skew-upwind scheme (Raithby, 1976) have been successful in increasing the accuracy of the solution, but all suffer from the boundedness problem; that is, the solutions display unphysical undershoots and overshoots in the regions of steep gradient, which can lead to numerical instability. In the practical turbulent calculations, the undershooting behavior of higher-order convection schemes may produce the negative value of turbulent quantities that should be always positive, such as the turbulent kinetic energy and the rate of dissipation of turbulent kinetic energy. Such a phenomenon can cause the numerical instability and occur in the analysis of turbulent natural convection or mixed convection of liquid metal flows in a liquid metal reactor.

Many higher-order bounded schemes, such as the SOUCUP scheme (Zhu and Rodi, 1991), the

HLPA scheme (Zhu, 1992), the SMARTER scheme (Shin and Choi, 1992) and the COPLA scheme (Choi et al. , 1995), have been developed to resolve the aforementioned boundedness problems. Recently Choi and Lee (1997) have evaluated these higher-order bounded schemes and have shown that the HLPA, SMARTER and COPLA schemes resulted in nearly the same solution behaviors in both accuracy and convergence, while the SOUCUP scheme is more diffusive than the other schemes. Thus, it suffices to test the SOUCUP and COPLA schemes in the present study.

In the present study, the higher-order bounded convection schemes are evaluated for transient oscillatory natural convection of a liquid metal. Among the various higher-order bounded schemes, the SOUCUP scheme and the COPLA scheme are chosen in the present study. The SOUCUP scheme is a composite of second-order upwind, central differencing and first-order upwind schemes and is second-order accurate. The COPLA scheme is a third-order accurate bounded scheme that employs the QUICK scheme in a certain range in the normalized variable diagram. The solutions of HYBRID scheme (Spalding, 1972) and QUICK scheme are also included for comparison.

The objectives of the present study are ; (1) a proper formulation of the Rhie and Chow scheme for unsteady flows, (2) evaluation of higher-order bounded convection schemes for simulation of oscillatory natural convection of liquid metal. The numerical results are compared with each other.

2. Mathematical Formulation

2.1 Governing equations

We consider a time-dependent, two-dimensional natural convection of liquid metal in a square cavity, shown in Fig. 1. The isothermal vertical walls are kept at constant but different temperatures, where the upper and lower walls are adiabatic. Initially the fluid is at the cold wall temperature. At time t=0, the temperature of one of the vertical walls is raised to a constant value

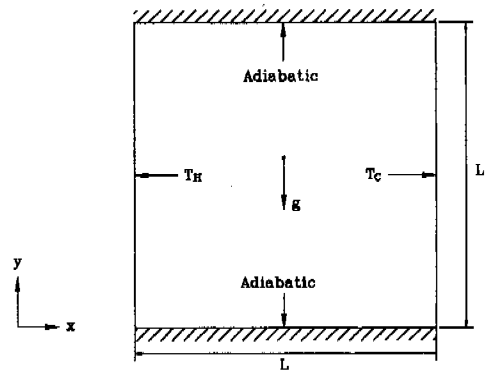


Fig. 1 Schematic of the cavity and coordinate system.

$T_H > T_C$. The fluid is assumed to be Newtonian with constant properties and the Boussinesq approximation is applied. The governing equations for the transport of mass, momentum and energy can be written as

$$\frac{\partial}{\partial x_i}(\rho u_i)=0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_j u_i)=-\frac{\partial P}{\partial x_i}+\frac{\partial}{\partial x_j}\left(\mu\frac{\partial u_i}{\partial x_j}\right)+\rho g_i\beta(T-T_0) \tag{2}$$

$$\frac{\partial}{\partial t}(\rho C_p T)+\frac{\partial}{\partial x_j}(\rho C_p u_j T)=\frac{\partial}{\partial x_j}\left(k\frac{\partial T}{\partial x_j}\right) \tag{3}$$

Using L, $(L/g\beta\Delta T)^{1/2}$, $(g\beta\Delta TL)^{1/2}$, and $\Delta T = T_H - T_c$ for the length, time, velocity and temperature scales, respectively, the non-dimensionalized governing conservation equations can be written as

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{4}$$

$$\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial x}+v\frac{\partial u}{\partial y}=-\frac{\partial P}{\partial x}+\frac{1}{\sqrt{Gr}}\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right) \tag{5}$$

$$\frac{\partial v}{\partial t}+u\frac{\partial v}{\partial x}+v\frac{\partial v}{\partial y}=-\frac{\partial P}{\partial y}+\frac{1}{\sqrt{Gr}}\left(\frac{\partial^2 v}{\partial x^2}+\frac{\partial^2 v}{\partial y^2}\right)+\theta \tag{6}$$

$$\frac{\partial \theta}{\partial t}+u\frac{\partial \theta}{\partial x}+v\frac{\partial \theta}{\partial y}=\frac{1}{\mathrm{Pr}\sqrt{Gr}}\left(\frac{\partial^2 \theta}{\partial x^2}+\frac{\partial^2 \theta}{\partial y^2}\right) \tag{7}$$

where the Grashof and Prandtl numbers are defined as

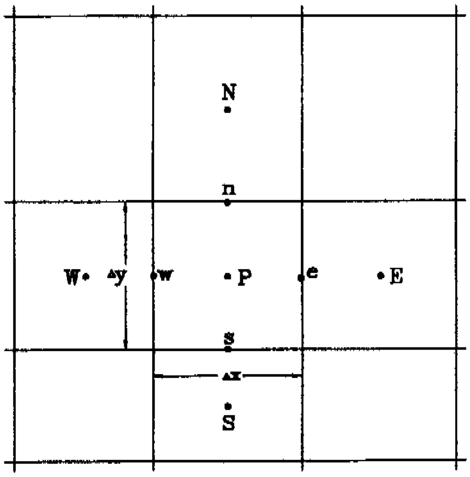


Fig. 2 Typical control volume and node notation.

$$Gr = \frac{g\beta \Delta T L^3}{\nu^2} \tag{8}$$

$$\Pr = \frac{\nu}{\alpha} \tag{9}$$

and $\theta = (T - T_0)/\Delta T$. The initial and boundary conditions are as follows ;

$$\begin{aligned} &u = v = \theta = 0 \quad t = 0 \\ &u = v = 0 \text{ on the walls } t \geq 0 \\ &\theta(0, y) = 1, \ \theta(1, y) = 0 \quad t \geq 0 \\ &\frac{\partial \theta}{\partial y} = 0 \text{ at } y = 0, 1 \quad t \geq 0 \end{aligned} \tag{10}$$

2.2 Discretization of transport equations

The computational domain is subdivided into finite number of control volumes as shown in Fig. 2 and all the variables are stored at the geometric center of each control volume cell. The transport equations are discretized using the finite volume approach (Patankar, 1980). The governing equations are integrated over the control volume and the convection terms are approximated by four different schemes. The unsteady term is treated by the backward differencing scheme. The resulting algebraic equation for a variable

$$A_P\phi_P = A_E\phi_E + A_W\phi_W + A_N\phi_N + A_S\phi_S + b_\phi \tag{11}$$

where b_ϕ is a source term for variable ϕ.

2.3 Momentum interpolation method

In the Rhie and Chow scheme, the momentum equations are solved implicitly at the center of the cell. The discretized momentum equations for velocity components can be written as

$$u_P = (H_u)_P + (D_u)_P (P_w - P_e)_P + (E_u)_P u_P^{n-1} + (1 - \alpha_u) u_P^{l-1} \tag{12}$$

$$v_P = (H_v)_P + (D_v)_P (P_s - P_n)_P + (E_v)_P v_P^{n-1} + (1 - \alpha_v) v_P^{l-1} \tag{13}$$

where

$$H_u = \alpha_u [\sum A_{nb}^u u_{nb} + (S_c^u \Delta V)] / A_P^u \tag{14}$$

$$H_v = \alpha_v [\sum A_{nb}^v v_{nb} + (S_c^v \Delta V)] / A_P^v \tag{15}$$

$$D_u = \alpha_u \Delta y / A_P^u \tag{16}$$

$$D_v = \alpha_v \Delta x / A_P^v \tag{17}$$

$$E_u = \frac{\alpha_u \rho \Delta V}{\Delta t} / A_P^u \tag{18}$$

$$E_v = \frac{\alpha_v \rho \Delta V}{\Delta t} / A_P^v \tag{19}$$

$$A_P^u = \sum A_{nb}^u - S_P^u \Delta V + \frac{\rho \Delta V}{\Delta t} \tag{20}$$

$$A_P^v = \sum A_{nb}^v - S_P^v \Delta V + \frac{\rho \Delta V}{\Delta t} \tag{21}$$

and α_u, α_v are the underrelaxation factors for u, v velocity components and the superscripts $n-1$, $l-1$ denote the previous time step and iteration level, respectively. The discretized momentum equations for the velocity component at the cell face, for example at the east face, can be written as follows.

$$u_e = (H_u)_e + (D_u)_e (P_P - P_E) + (E_u)_e u_e^{n-1} + (1 - \alpha_u) u_e^{l-1} \tag{22}$$

In the present modified Rhie and Chow's scheme, this velocity component is obtained explicitly through the interpolation of momentum equations for the neighbouring cell-centered velocity components. Following assumptions are introduced to evaluate this cell face velocity component.

$$(H_u)_e \approx f_e^+ (H_u)_E + (1 - f_e^+) (H_u)_P \tag{23}$$

$$\frac{1}{(A_P^u)_e} \approx \frac{f_e^+}{(A_P^u)_E} + \frac{(1 - f_e^+)}{(A_P^u)_P} \tag{24}$$

where f_e^+ is the geometric interpolation factor defined in terms of distance between nodal points. Similar assumptions can be introduced for evaluation of the velocity component at the north face.

Using the above assumption, Eq. (22) can be written as follows, with the E_u term expressed explicitly.

$$
\begin{aligned}
u_e = & [f_e^+ u_E + (1-f_e^+) u_P + (D_u)_e (P_P - P_E) \\
& - f_e^+ (D_u)_E (P_w - P_e)_E \\
& - (1-f_e^+) (D_u)_P (P_w - P_e)_P)] \\
& + (1-\alpha_u) [u_e^{l-1} - f_e^+ u_E^{l-1} - (1-f_e^+) u_P^{l-1}] \\
& + \frac{\alpha_u \rho}{\Delta t} \left[\frac{(\Delta V)_e}{(A_P^u)_e} u_e^{n-1} - f_e^+ \frac{(\Delta V)_E}{(A_P^u)_E} u_E^{n-1} \right. \\
& \left. - (1-f_e^+) \frac{(\Delta V)_P}{(A_P^u)_P} u_P^{n-1} \right]
\end{aligned}
\tag{25}
$$

The expression in the first bracket of the right hand side is the original Rhie and Chow's scheme. Majumdar (1988) has revealed that the converged solution was relaxation factor-dependent if the expression in the second bracket was omitted. For the same reason, omission of the last bracket leads to a converged solution which is dependent on the time step size. To the present authors' knowledge, nobody has mentioned in the literature the last term, which comes from the unsteady term. Although the above two terms are relatively small in the practical calculations and do not influence the accuracy of the converged solution significantly, this feature that the converged solution is dependent on the relaxation factors and time step size is obviously undesirable. Equation (25) indicates that the previous time step and the iteration values of cell face velocity components as well as those of centered velocity components should be stored in order to obtain the converged solutions which are independent of time step size and relaxation factors.

3. Results and Discussions

The modified Rhie and Chow scheme described in the previous section is implemented in a general purpose code designed to solve the fluid flow and the heat transfer in complex geometries. The SIMPLE (Patankar, 1980) algorithm is employed for pressure-velocity coupling.

The calculations are performed for $Gr=10^7$, Pr $=0.005$ employing 42×42 and 82×82 nonuniform grids. The numerical grids used in the present study are the same as those reported in Hortmann et al. (1992). Dimensionless time step of 1/80 is used for all calculations and this time step size is small enough to resolve the oscillatory transient behaviour. Iterations are performed for each time step until the maximum of the absolute sum of dimensionless residuals of momentum equations, energy equation and pressure correction equation is smaller than 10^{-6}. Relaxation factor of 0.7 is used for momentum equations and 1.0 is used for the energy equation. It takes about 72 hours on our computer (Pentium Pro 200MHz) to obtain a transient solution up to dimensionless time of 37.5 when the QUICK scheme with 82×82 grids are employed.

Mohamad and Viskanta (1991) have solved this problem using the central difference scheme. Three different numerical grids, 42×42, 62×62, 82×82, were tested and they have shown that the solution by 82×82 grids was nearly grid independent. The magnitude and trend of average Nusselt number at the hot wall by the QUICK scheme employing 82×82 grids is very similar to their grid independent solution and this solution can be considered as a nearly grid independent solution. Thus, further grid refinement tests are not performed due to requirement of excessive computational efforts. The numerical solutions by the other schemes are evaluated using this solution as a basis solution.

During the reviewing process, one reviewer questioned that the present problem ($G_r=10^7$, Pr $=0.005$) could be considered as a laminar flow. To present author's knowledge, the stability study for the natural convection of liquid metal in a cavity for the case of Pr$=0.005$ is not reported in any literature. Muller et al. (1984) has reported a stability study for natural convection of liquid metal Ga (Pr$=0.02$) in a cylinder. They have explained the development of natural convection of liquid metal in four stages, no flow, steady laminar flow, unsteady periodic laminar flow and unsteady turbulent flow. The stability diagram by Muller et al. (1984) and the present calculated results show that the present problem belongs to the stage of unsteady periodic laminar flow and can be solved by laminar flow equations as was done by Mohamad and Viskanta (1991) and Cless and Prescott (1996).

Figure 3 shows the transient average Nusselt

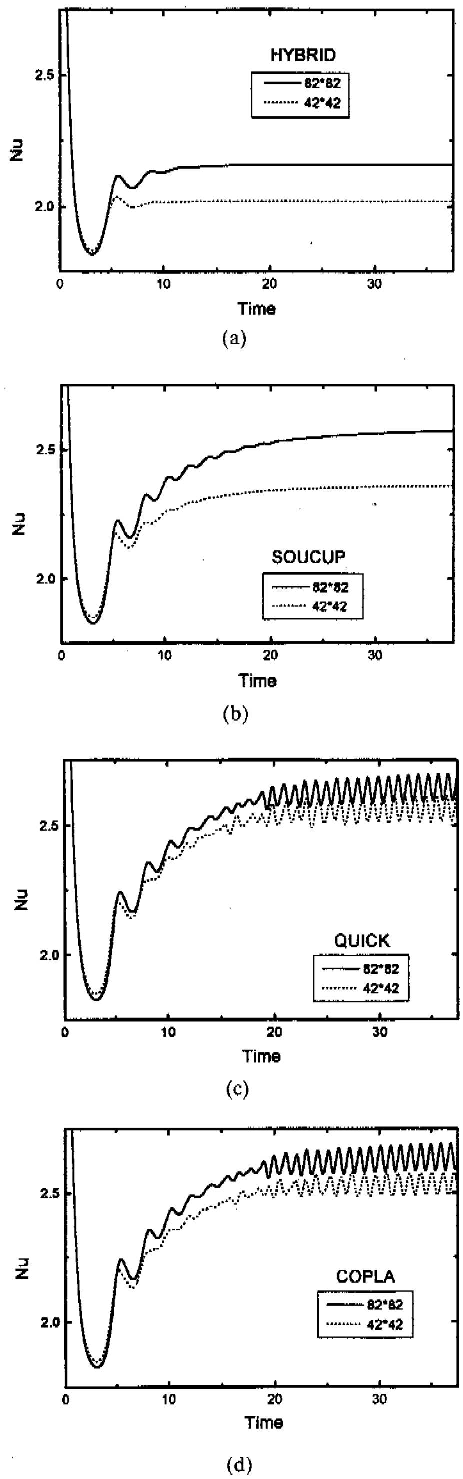
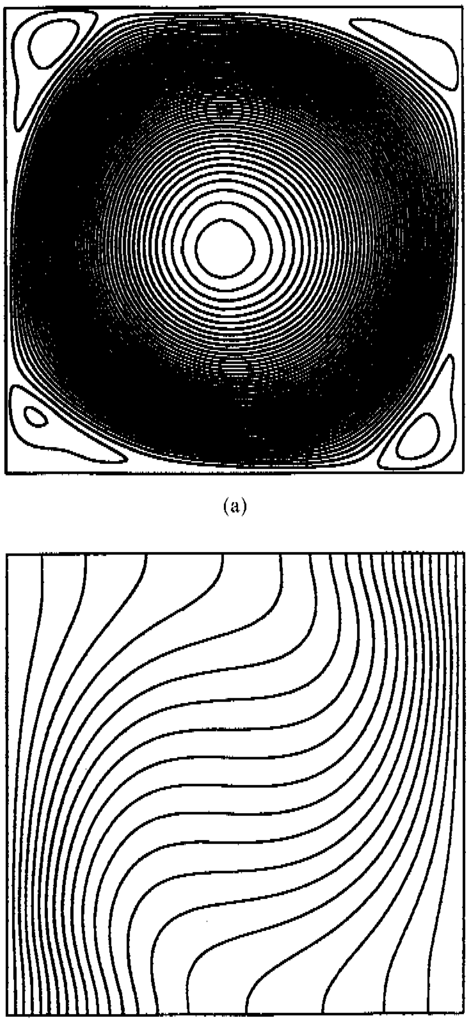


Fig. 3 Transients of average Nusselt number at the hot wall($Gr = 10^7$, $\Pr = 0.005$) : (a) HYBRID, (b) SOUCUP, (c) QUICK, (d) COPLA.

number at the hot wall predicted by four different convection schemes. We can observe that the HYBRID and SOUCUP schemes result in the steady state solutions. These two schemes are not capable of predicting the oscillatory behaviour, even if the numerical grids are increased to 82×82. The HYBRID scheme underpredicts the average Nusselt number severely. The prediction does not improve much with grid refinement. The SOUCUP scheme predicts the average Nusselt number much better than the HYBRID scheme, however, it fails to predict the oscillatory behaviour. It is noted that the SOUCUP scheme is a composite of upwind, second order upwind and central difference scheme and is second order accurate. The QUICK and the COPLA schemes predict the oscillatory behaviour of the average Nusselt number well. These predictions by the QUICK and the COPLA schemes are very similar to those reported by Mohamad and Viskanta (1991) which have been obtained by the central difference scheme. The predictions by both schemes are nearly the same, while the QUICK scheme results in slightly better results when the grid is coarse (42×42). It is not a surprising result if we note that the bounded scheme COPLA employs the QUICK scheme in a certain range in the normalized variable diagram. The results show that the bounded scheme COPLA is as accurate as the QUICK scheme and the QUICK scheme does not show wiggling in the present problem.

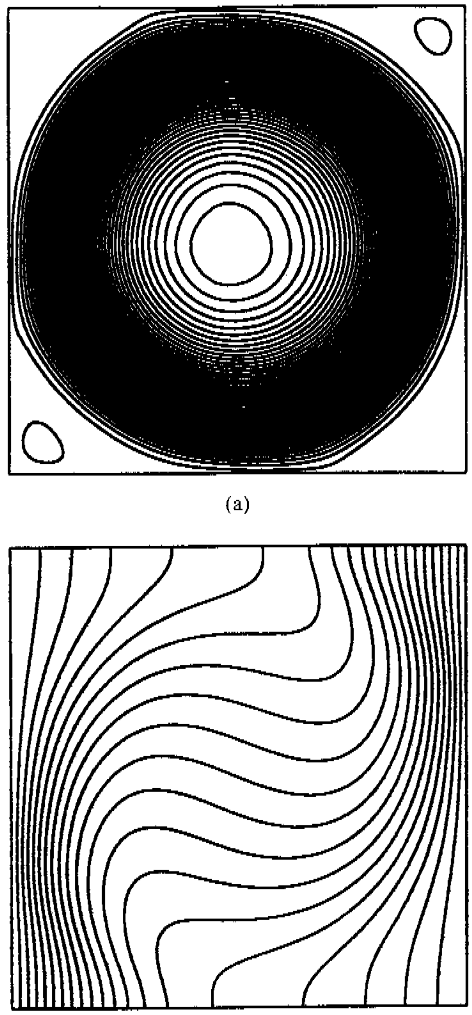
Figure 4 and 5 show the predicted streamlines and isothermal lines by the HYBRID and SOUCUP schemes in the final stages of steady state. Only the results for 82×82 grids are presented. The streamlines predicted by the HYBRID scheme are rather square shaped compared with those by the SOUCUP scheme. The HYBRID scheme predicts rather large vortices at the four corners and it is found that these vortices are weak and do not change with time. The streamlines predicted by the SOUCUP scheme are nearly circular. There are two very small vortices at upper-right and bottom-left corners. It is also checked that these vortices do not vary with time. Differences in flow structure between the two



(a)

(b)

Fig. 4 Streamlines and isotherms predicted by HYBRID($Gr=10^7$, Pr=0.005) ; (a) streamlines, (b) isotherms.



(a)

(b)

Fig. 5 Streamlines and isotherms predicted by SOUCUP($Gr=10^7$, Pr=0.005) ; (a) streamlines, (b) isotherms.

schemes affect the temperature distributions. The temperature distributions predicted by the two schemes are significantly different.

Figure 6 shows the unsteady motion of streamlines during one cycle of oscillation predicted by the COPLA scheme employing 82×82 grids. The streamlines reveal nearly periodic growth and decay of corner vortices. The evolution of corner vortices during a cycle of oscillation can be described as follows. The evolution of vortices begins at the upper-right and bottom-left corners where the temperature gradient is large (t=35.3135). The upper-right and bottom-left vortices appear first, and the vortices at the other corners also evolve (t=35.4760). Then the strength of the vortices increases (t=35.6510) and the corner vortices shear with the main vortices (t=35.8010). The strength of the corner vortices is weakened and split into small vortices (t=35.9510). Then the corner vortices disappear and evolve into main vortices (t=35.1510). This ends one cycle of the evolution process. When these predictions are compared with the predictions of streamlines by the HYBRID and SOUCUP

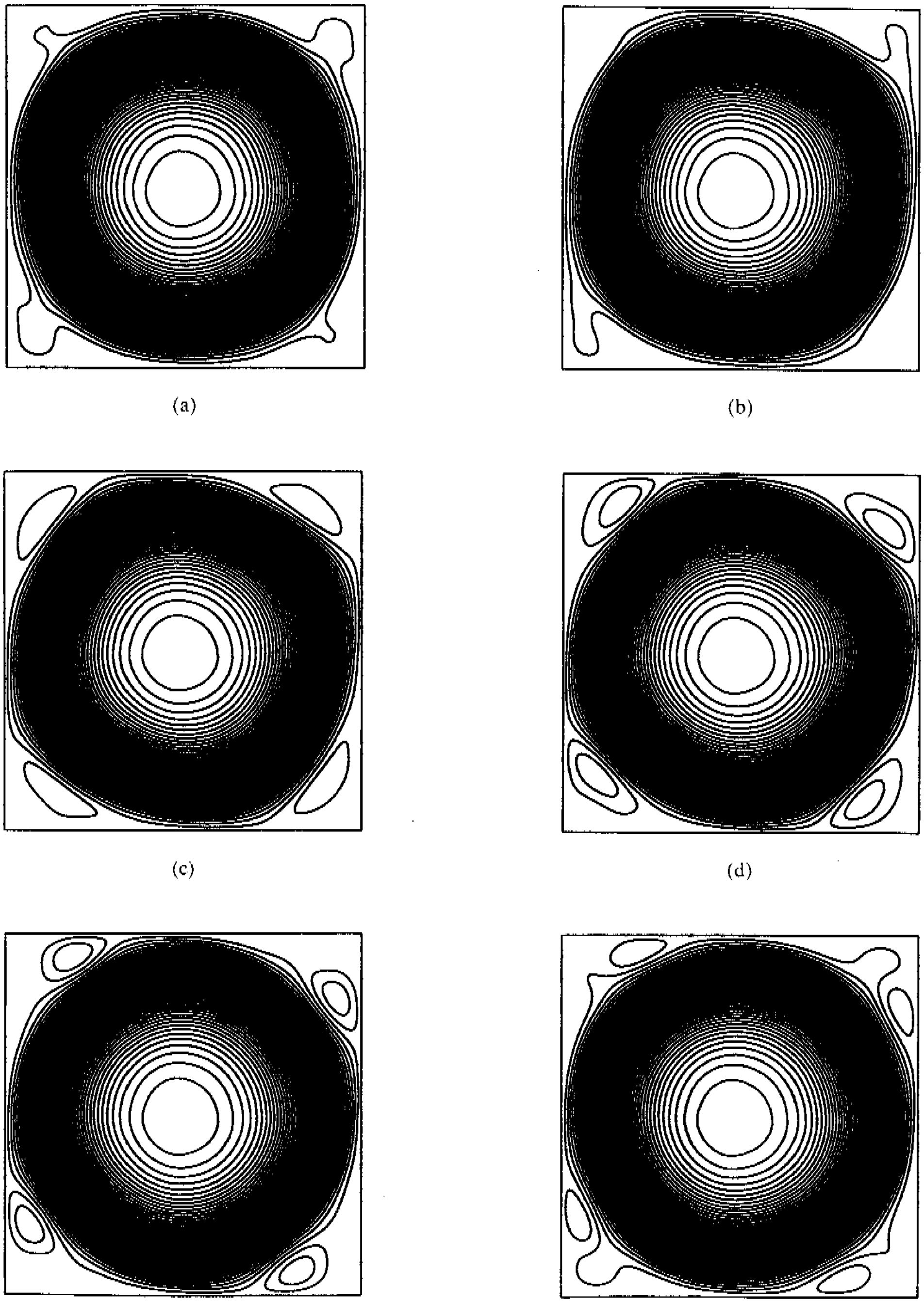
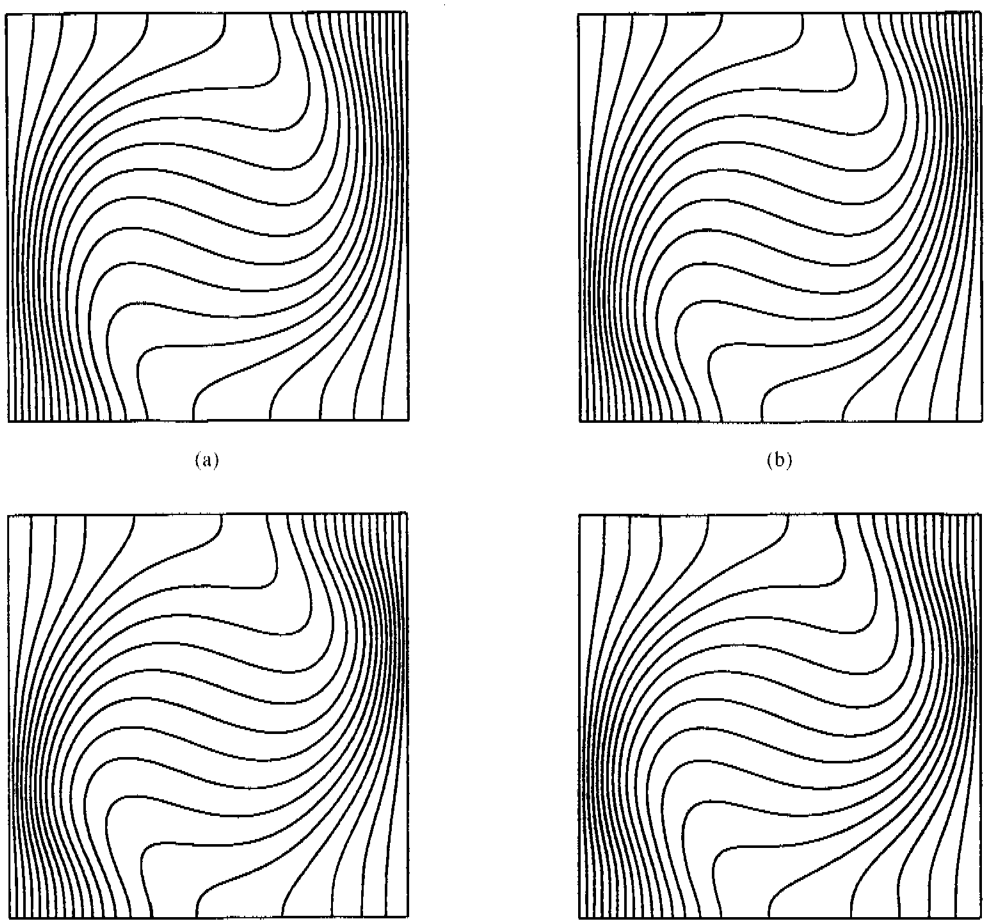


Fig. 6 Streamlines during one cycle of oscillation predicted by COPLA ($Gr=10^7$, $Pr=0.005$) : (a) t=35.1510, (b) t=35.3135, (c) t=35.4760, (d) t=35.6510, (e) t=35.8010, (f) t=35.9510.

schemes, the oscillation of the average Nusselt number is due to the unsteady motion of corner vortices.

Figure 7 shows the plots of isothermal lines during one cycle of oscillation predicted by the COPLA scheme employing 82×82 grids. The



(a) (b)

(c) (d)

Fig. 7 Isotherms during one cycle of oscillation predictred by COPLA ($Gr=10^7$, Pr=0.005) ; (a) t=35.1510, (b) t=35.4135, (c) t=35.6510, (d) t=35.8760.

temperature field oscillates, however, the magnitude of temperature oscillation is small and no significant change during a cycle is observed in the contour plot.

The plots of streamlines and isotherms predicted by the QUICK scheme are not presented here since they are essentially the same as those of the COPLA scheme, which can be conjectured from the results shown in Fig. 3 (c) ~ (d).

4. Conclusions

The use of the momentum interpolation method and the evaluation of higher-order bounded convection schemes for the simulation of oscillatory natural convection of low Prandtl number fluids are studied. A proper formulation of Rhie and Chow scheme for unsteady flows is presented. Four convection schemes are tested for the natural convection of liquid metal in a square cavity in the case of $Gr=10^7$, Pr=0.005 by employing 42×42 and 82×82 nonuniform grids. The results of numerical experiments conducted by the present study show that the HYBRID and the SOUCUP schemes should not be used for the prediction of oscillatory natural convection of liquid metal since they fail to predict the experimentally observed oscillatory motion. The QUICK scheme and the central difference scheme tested by Mohamad and Viskanta (1989) are capable of predicting the oscillatory motion. However, these two schemes are unbounded and can cause numerical instability in the turbulent flow simulations. The results of present study and those of Choi et al. (1995) show that the COPLA scheme is as accurate as the QUICK scheme, while preserving the boundedness of the problem. Thus, the higher-order bounded scheme like COPLA scheme can be used confidently for practical simulation of both laminar and turbulent natural convection of liquid metal such as the decay heat removal in a liquid metal reactor or the thermohydraulic analysis of severe accident in a nuclear power plant (Lee and Park, 1998).

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