R & D NOTES

Three-Dimensional Numerical Analysis of Natural Convection in an Inclined Channel with a Square Cross Section

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Many articles on natural convection in enclosures have appeared recently, primarily because of applications in solar heating. Most of these studies involve geometries or boundary conditions quite different than those of this paper.

It has been known for some time (see, for example, Davis, 1967; Ozoe, 1971; Catton, 1972) that the stable mode of circulation in a long, square channel, heated from below, is a series of roll cells whose axes are parallel to the heated surface and perpendicular to the long dimension of the channel. The width of each fluid cell has been observed to be approximately equal to the height of the channel. The y-z surfaces resist the circulation at the ends of the roll cells and introduce some three dimensionality. Davis (1967) computed critical Rayleigh numbers in various finite rectangular enclosures with infinitely conducting side walls, and Catton (1972) carried out improved calculations for perfectly insulated side walls and many aspect ratios. Ozoe et al. (1976) were apparently the first to take three dimensionality into account for Rayleigh numbers above the critical value. They showed that for Ra = 2 600 to 8 000 and Pr = 10, the fluid particles trace a closed, concentric helix in each

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TABLE 1. COMPUTED RESULTS

$Ra = 4\,000, Pr = 10, \Delta X = \Delta Y = \Delta Z = 0.125$

Degrees of inclination	Nu at $Z = 0.5$ calc.	Nu at $Z = 0.5$ corr.	ψ_x	ψ_y (at $X = Y = Z = 0.5$)	ψ_z	$\lvert\psi\rvert$	Mode
0.0	1.80	1.59	4.20	0.00	0.000	4.20	A
2.0	1.78	1.57	3.94	1.33	0.149	4.16	B
3.0	1.70	1.49	3.23	2.39	0.188	4.02	B
4.0	1.61	1.41	0.00	3.74	0.000	3.74	C
6.0	1.65	1.44	0.00	3.91	0.000	3.91	C
10.0	1.71	1.50	0.00	4.19	0.000	4.19	C
30.0	1.89	1.68	0.00	4.92	0.000	4.92	C

Mode
A A series of three-dimensional roll cells with their axes horizontal and perpendicular to the long dimension of the channel.
B A series of three-dimensional, oblique roll cells.
C A single, two-dimensional roll cell with its axis in the long dimension of the channel.

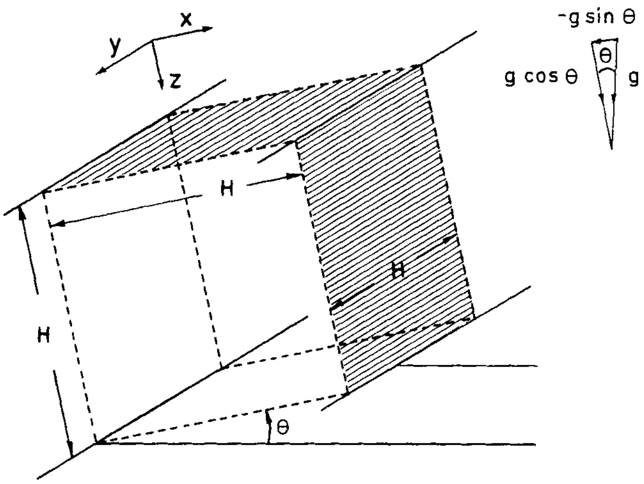

Fig. 1. Geometry of a series of roll cells in a horizontal square channel. Geometrical configuration for a fluid cell in an inclined square channel.

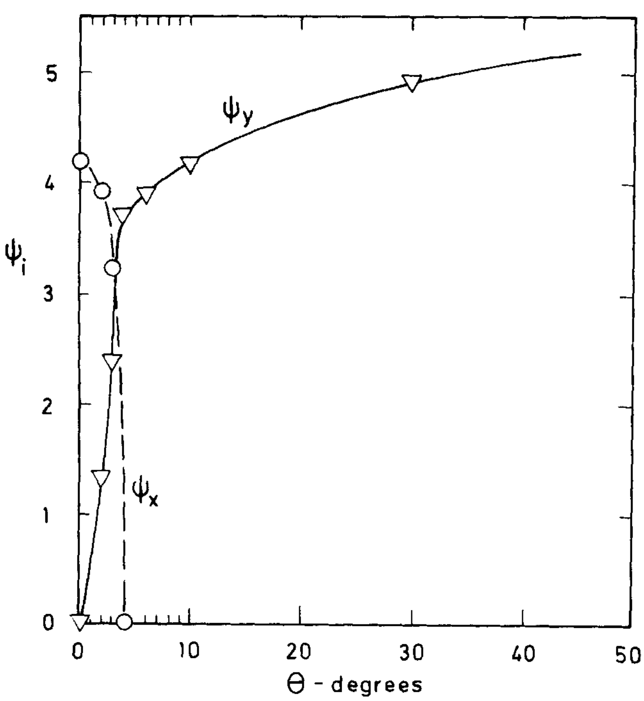

Fig. 2. Vector potential at $X = Y = Z = 0.5$ as a function of angles of inclination. $Ra = 4\,000$, $Pr = 10$, $\Delta X = \Delta Y = \Delta Z = 0.125$.

half of the roll cells, with an average axial velocity equal to about 5% of the radial velocity. Comparison of their computed average Nusselt numbers for the square channel with those for two-dimensional cells indicates that the effect of the drag is quite significant. Their results incorporate some unknown numerical error due to the use of a finite grid size, but these two observations are undoubtedly valid even so.

Ozoe et al. (1974, 1975) observed experimentally that inclination of the heated surface of a long channel about the long axis, as illustrated in Figure 1, produced first a decrease and then an increase in the rate of heat transfer. During the regime of decreasing heat transfer, the circulation pattern was observed to change significantly, even though the fluid cell boundaries did not shift. For inclinations beyond that corresponding to the minimum rate of heat transfer, the series of roll cells degraded abruptly to a single roll cell with its axis in the long dimension of the channel. This roll cell is, of course, truly two dimensional. These studies were for $Ra = 3\,800$, $Pr = 5\,580$; $Ra = 4\,950$, $Pr = 5\,220$; $Ra = 11\,000$, $Pr = 2\,690$; $Ra = 46\,500$, $Pr = 4\,870$; and $Ra = 90\,600$, $Pr = 4\,690$. Two-dimensional, finite-difference solutions, extrapolated to zero grid size, were obtained for $Ra = 2\,000$, $3\,000$, $4\,000$ and $8\,000$ and $Pr = 10$.

The objective of the present investigation was to develop theoretical solutions for an inclined square channel in the three-dimensional regime and in particular to

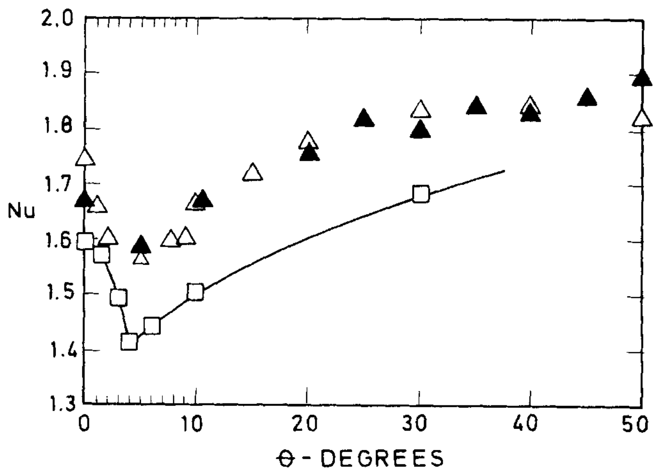

Fig. 3. Comparison of experimental and computed rates of heat transfer. □—this work-theoretical, $Ra = 4\,000$, $Pr = 10$, $\Delta X = \Delta Y = \Delta Z = 0.125$, but extrapolated to zero. △—experimental, $Ra = 4\,800$ to $4\,950$, $Pr = 5\,220$ (increasing θ). ▲—experimental, $Ra = 4\,800$ to $4\,950$, $Pr = 5\,220$ (decreasing θ).

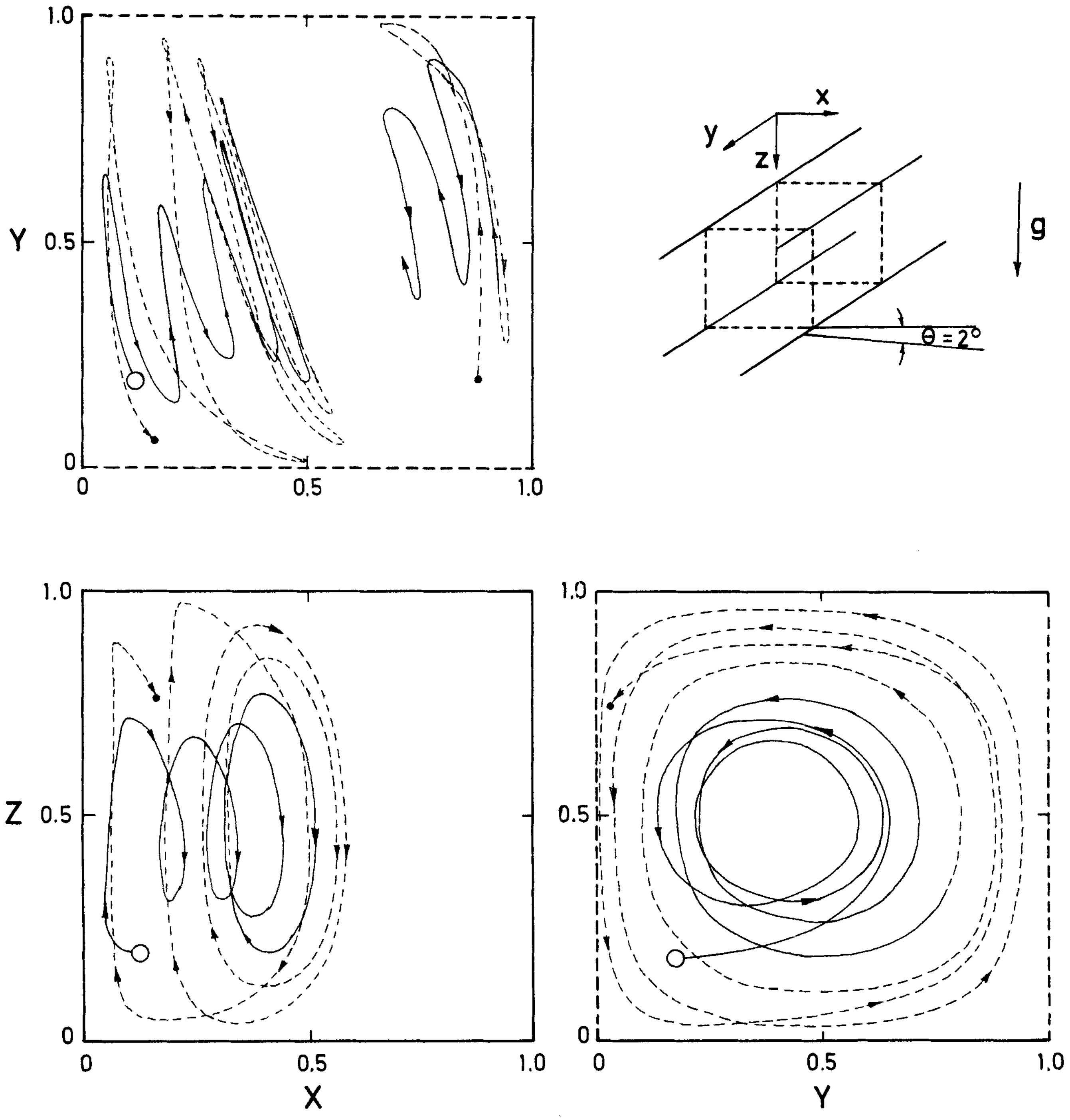

Fig. 4. Fluid particle path with a 2 deg inclination. $Ra = 4\,000$, $Pr = 10$, $\Delta X = \Delta Y = \Delta Z = 0.125$. ○—starting point ($X = 0.125$, $Y = Z = 0.1875$). ●—$\tau = 2.5$.

determine the critical angle for transition to the two-dimensional regime. After the work reported herein was completed, three-dimensional calculations were carried out by Ozoe et al. (1977) for a 2 × 1 rectangular channel for the special and limited purpose of interpreting tri-directional photographs of the flow patterns. Since the equivalent mathematical model and method of computation are described in detail therein, they will only be summarized here.

MATHEMATICAL MODEL AND METHOD OF SOLUTION

In accordance with the above experiments, the lower surface was postulated to be at a uniform temperature T_h, the upper surface at a lower uniform temperature T_c, and the side walls of the channel to be perfectly insulated. In accordance with the observations mentioned above, the fluid cells were postulated to be cubical. The Boussinesq approximations of negligible dissipation and negligible variation in physical properties, other than the density in the buoyant term, were also postulated.

The partial differential equations describing the conservation of mass, energy, and momentum were written in terms of the vector potential and the vorticity. They were solved numerically.

Essentially the same computational scheme as developed by Ozoe et al. (1976) was used herein. The sides of the cubical cell were divided into eight segments for the finite-difference calculations owing to the limited memory of the available computer (NEAC 2200/500 at the Okayama University Computing Center). A dimensionless time step $\Delta\tau = 0.001$ was used. Doubling the number

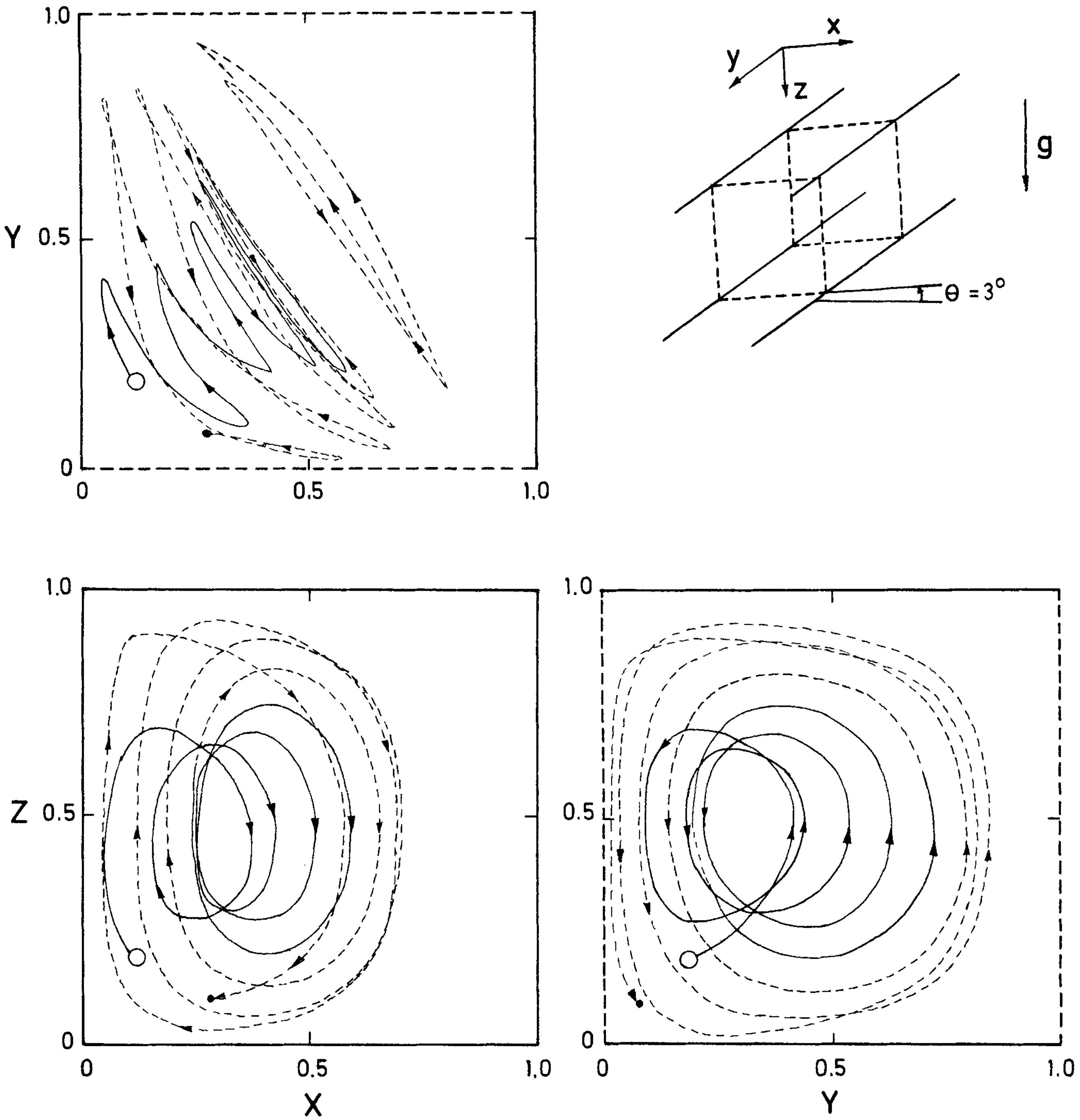

Fig. 5. Fluid particle path with a 3 deg inclination. Ra = 4 000, Pr = 10, $\Delta X = \Delta Y = \Delta Z = 0.125$. ○—starting point ($X = 0.125$, $Y = Z = 0.1875$). ●—$\tau = 2.325$.

of grid points would increase the memory requirement by a factor of 8 and would also require a smaller $\Delta\tau$, hence increasing the computing time greatly. The finite difference representation of the energy and vorticity balances [Equations (7) and (8) of Ozoe et al., (1977)] was solved using the three-dimensional ADI (alternating direction implicit) method of Brian (1961). The three-components of the vector potential were obtained at each time step using Equation (9) of Ozoe et al. (1977) with a fictitious, unsteady term as proposed by Samuels and Churchill (1967) and recently discussed by Mallinson and deVahl Davis (1973). Each time step required 5 to 20 s of computer time. The number of steps required for a satisfactory convergence to the steady state ranged from less than 200 for the same mode to over 10 000 for a radical change in mode, as discussed below.

NUMERICAL RESULTS

The calculations were carried out for Ra = 4 000, Pr = 10, and $\Delta X = \Delta Y = \Delta Z = 0.125$, with only the angle of inclination as a variable. The correlation for the error due to the use of a finite grid size which was developed by Ozoe (1971) for two-dimensional calculations was used to correct Nu. The computed and corrected values of the average Nusselt number at the central plane of the cell and the three components and absolute value of the dimensionless vector potential at the center of the cell are listed in Table 1.

The numerical results were obtained as the steady state was approached after a step change in Ra or θ. The solution for a horizontal channel converges rapidly (in less than 200 time steps) after a change in Ra from 3 700 to 4 000. On the other hand, the rate of convergence after

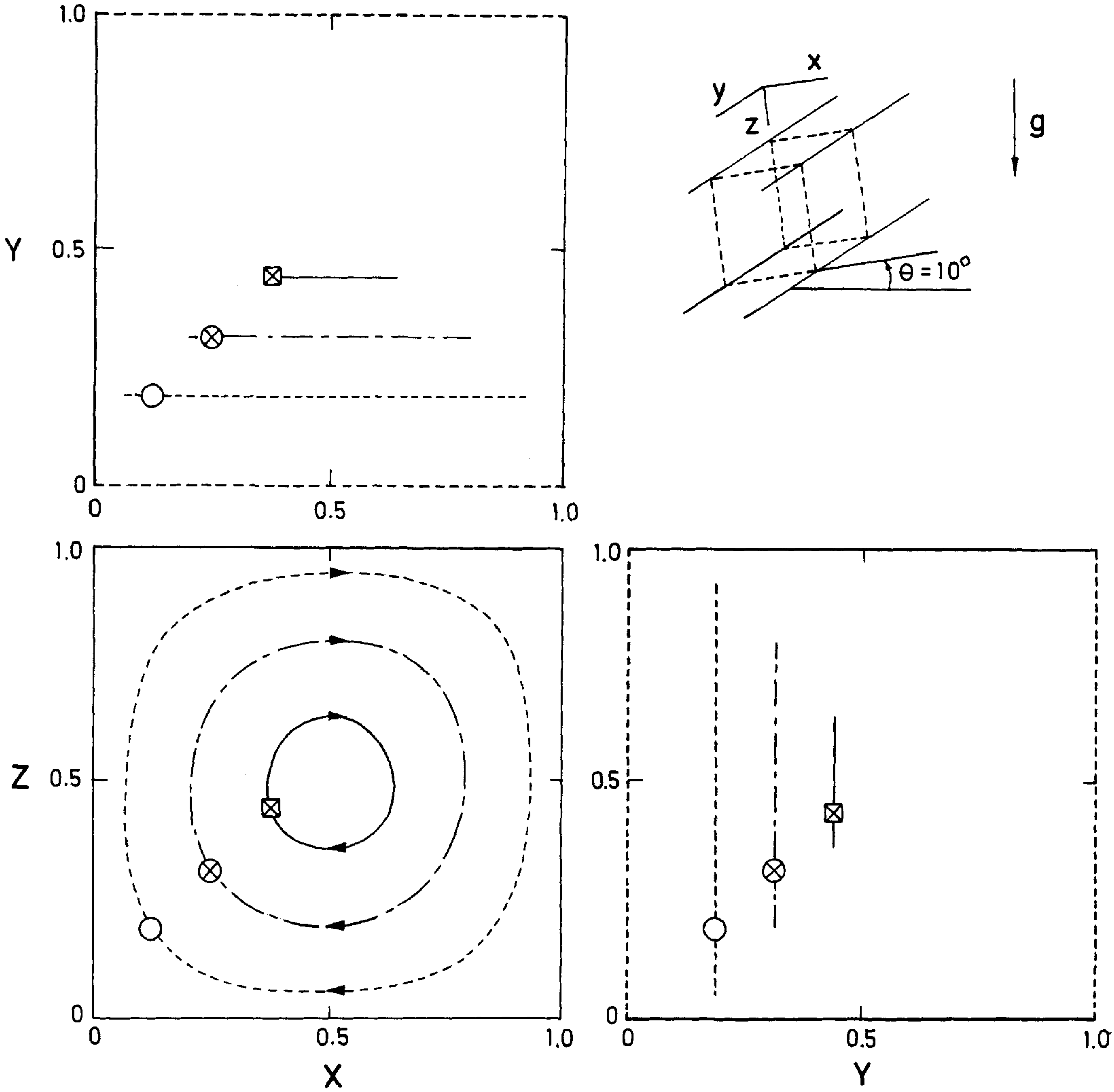

Fig. 6. Fluid particle path with a 10 deg inclination. Ra = 4 000, Pr = 10, $\Delta X = \Delta Y = Z = 0.125$. ○—starting point ($X$ = 0.125, $Y = Z = 0.1875$). ⊗—starting point (X = 0.25, $Y = Z = 0.3125$). ⊠—starting point (X = 0.375, $Y = Z = 0.4375$).

a change in the angle of inclination from 0 to 2 deg is very slow (more than 900 time steps are required) because the mode of circulation has to change from roll cells normal to the long dimension of the channel to oblique cells. For a change from 2 to 4 deg, the mode of circulation changes radically, from a series of three-dimensional, oblique roll cells to a single, two-dimensional, longitudinal roll cell. The solution did not quite attain a steady state in 10 440 time steps. This much computation cannot be justified for every case but reveals that such a drastic transition can be simulated. The reverse transition can also be computed. A step change from 4 back to 3 deg after 400 time steps resulted in rapid reversion to the oblique cells. Reversion after attainment of the steady state would, of course, take longer.

To avoid such excessive computer usage in determining the angle of transition, the calculations were instead first carried out for 30 deg of inclination. For such a large inclination, the stable mode is unquestionably a two-dimensional roll cell. This solution was used as a starting condition for 10, 6, and 4 deg. Rapid convergence was attained. Such a technique was used to construct Figure 2 in which the steady state values of the X and Y components of the dimensionless vector potential are plotted vs. the angle of inclination. The crossover in the values of ψ_x and ψ_y at about 3.2 deg and the rapid decrease in ψ_x to zero with a further increase in the angle of inclination indicates the attainment of two-dimensional motion. The relative magnitude of ψ_x and ψ_y, therefore, appears to be a simple and useful criterion for the critical angle of transition from the oblique mode to the two-dimensional mode or vice versa. Exhaustive calculations across the transition are thus avoided.

The computed and corrected values of the average Nusselt number for Ra = 4 000 with Pr = 10 are compared with the experimental values of Ozoe et al. (1974)

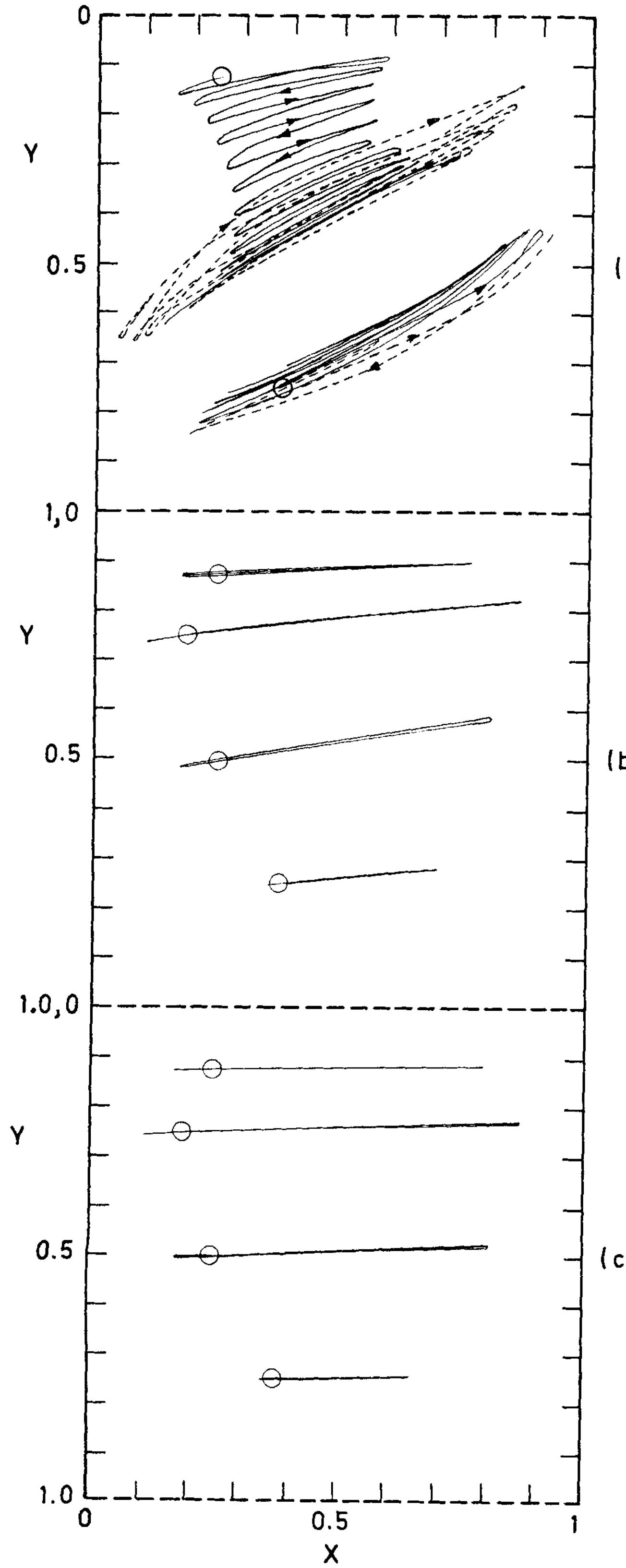

Fig. 7. Fluid particle path at transient states after a change in angle of inclination from 2 to 4 deg. $Ra = 4\,000$, $Pr = 10$, $\Delta X = \Delta Y = \Delta Z = 0.125$. (a) $\tau = 2.404$. (b) $\tau = 6.422$. (c) $\tau = 10.44$.

for $Ra = 4\,800$ to $4\,950$, with $Pr = 5\,200$ in Figure 3. The three-dimensional solution clearly predicts the angle of transition and the correct behavior for angles less than 3.2 deg, whereas the two-dimensional solution for Nu (not shown) continues to decrease.

The decreasing rate of heat transfer with increasing angle of inclination up to 3.2 deg and the subsequent increasing rate of heat transfer are associated with the varying rate of circulation. The rate of circulation can be characterized by the absolute value of the vector potential at $X = Y = Z = 0.5$. Such values are included in Table 1 and may be seen to vary directly with the average Nusselt number.

Figure 4 shows the traces in the X, Y, and Z planes of the path of a fluid particle for 2 deg of inclination. This particle, starting from $X = 0.125$, $Y = Z = 0.1875$, traces a skewed helix with a small radius of gyration. At about $X = 0.4$, the axial component of the motion decreases and reverses direction, while the radius of gyration increases to a larger value as the particle proceeds toward $X = 0$. The solid point indicates a dimensionless time span $\tau = 2.5$. Part of a particle path in the other half of the fluid cell is also shown. The solid and hatched lines indicate the forward and backward flows but actually constitute parts of a single, continuous line.

Figure 5 illustrates a fluid particle path for an inclination of 3 deg. The axis of gyration further approaches the direction of the diagonal of the base of the cubical cell. A helix is again apparent. Figure 6 shows several particle paths for 10 deg of inclination. The circulation is clearly two dimensional, with its axis in the long (Y) dimension of the channel, and provides some confirmation of the accuracy of the method of computing the fluid particle path.

Figure 7 shows the X-Y streak lines at three transient states after the step change of the angle of inclination from 2 to 4 deg. The initial flow pattern is that of Figure 5 but with the reverse direction of circulation. The circulation passes through a state close to that of Figure 5, then through Figures 7*a*, *b*, and *c* and would eventually reach a steady state close to that of Figure 6.

The direction of the axis of rotation for various angles of inclination is shown schematically in Figure 8. The

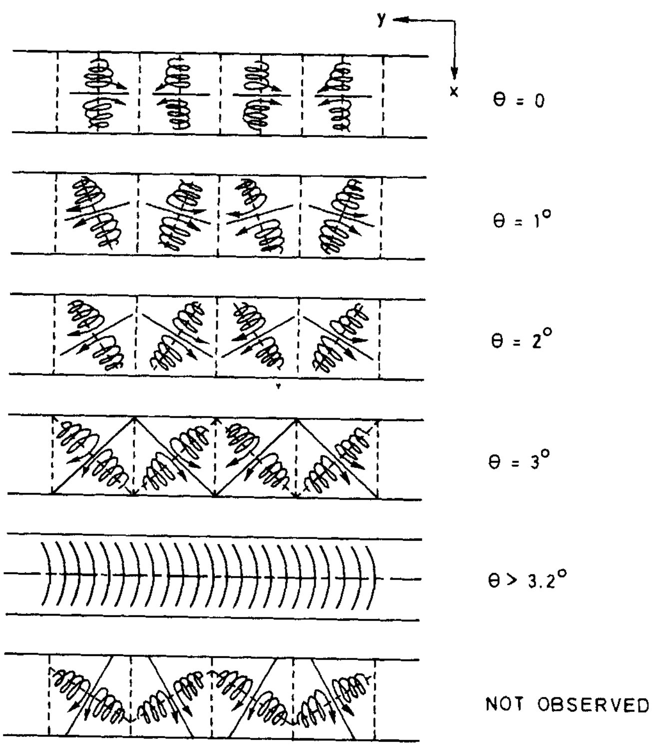

Fig. 8. Sketch of stable circulation patterns—top view. ------------ axis of circulation; cell interface. ———— half cell interface.

axis starts in the X direction for the horizontal case, shifts up to the X-Y diagonal line at about 3.2 deg of inclination, and then shifts abruptly to the Y direction for all higher angles. A stable roll does not appear to exist with its axis terminating in the planes of symmetry. This figure indicates why a half cell interface has never been observed from the long side of a square channel.

Comparable plots are given by Ozoe et al. (1976) for a horizontal channel and by Ozoe et al. (1977) a rectangular, inclined channel.

CONCLUSIONS

The three-dimensional model and numerical method utilized herein reproduce the experimentally known stable states and angle of transition for natural convection in a long, square channel, heated from below and rotated about the long axis of the channel.

The circulation pattern for no inclination of the channel is a series of quasi two-dimensional roll cells with their axes parallel to the heated surface and perpendicular to the long dimension of the channel. These fluid cells are essentially cubical. As the heated surface is inclined from the horizontal, the axes of the roll cells remain parallel to the heated surface but begin to rotate toward the long axis of the channel. The circulation also becomes increasingly three dimensional. At 3.2 deg of inclination of the heated surface, the axes of the roll cells are inclined 45 deg from the long dimension. As the angle of inclination of the heated surface is increased above 3.2 deg, the mode of circulation shifts abruptly to a single, truly two-dimensional roll cell with its axis parallel to the long dimension of the channel.

These transitions are reversed as the angle of inclination of the heated surface is decreased. Extensive computer time is required to trace the transition between multiple roll cells and a single roll cell. The angle of transition can, however, be determined with much less computation from a plot of the components of the vector potential for a series of stationary states on both sides of the transition.

The average Nusselt number first decreases as the heated surface is inclined relative to the horizontal, owing to the increased skewness of the roll cells and the associated decrease in their rate of circulation. At 3.2 deg, the average Nusselt number attains its minimum value. As the angle of inclination is further increased, the Nusselt number increases in correspondence to the increased rate of circulation of the single, two-dimensional roll cell.

The absolute values of the average Nusselt number, as computed, are somewhat in error owing to the economic necessity of using only a single, large grid size. These values were therefore corrected to zero grid size on the basis of prior two-dimensional calculations for a series of decreasing grid sizes. The corrected values are in good agreement with experimental observations. These results represent a significant, intrinsic improvement over prior solutions for two-dimensional or linearized models which are unable to predict the behavior in the three-dimensional regime even qualitatively.

Denny and Clever (1974) compared the ADI finite-difference method and the Galerkin expansion method for the calculation of two-dimensional natural convection. They concluded that the Galerkin method may require less computer time if an accuracy of 2 or 3% is acceptable but that the preparation time and storage requirements are much greater. They apparently did not consider extrapolation to zero grid size from calculations for a few gross grids as suggested by Chu and Churchill (1977) or extrapolation of the ADI calculation to steady state as suggested by Schoenherr and Churchill (1970). These two techniques may make the finite-difference method even more attractive.

Since the completion of this work, a report by Mallinson and deVahl Davis (1975) on three-dimensional calculations for natural convection in enclosures has come to our attention. It is apparent that they independently concluded that the best method of portraying the motion was through streak lines. However, they chose to use isometric projections rather than traces on the three orthogonal planes as we did herein and in Ozoe et al. (1976).

The computed results for $Pr = 10$ are presumed to be a good approximation for all $Pr >> 1$, based on experimental results for infinite horizontal plates. It is planned to study the actual dependence on Pr in the continuation of this work.

The streak lines computed by Ozoe et al. (1977) for a 2×1 channel has the same qualitative character as that illustrated herein but is more distorted. Also, the angle of inclination for transition changes decisively. Transition occurs when the oblique roll cells broach the diagonal plane of the channel. For an aspect ratio of 2.0, an inclination of 7.0 deg is required as compared to 3.2 deg for the square channel.

NOTATION

g = acceleration due to gravity
H = height and width of channel, length of fluid cell
k = thermal conductivity
Nu = mean Nusselt number $= qH/k(T_h - T_c)$
Pr = Prandtl number $= \nu/\alpha$
q = heat flux
Ra = Rayleigh number $= g\beta(T_h - T_c)\ H^3/\nu\alpha$
t = time
T_c = temperature of cold plate
T_h = temperature of hot plate
x = coordinate (across channel with $\theta = 0$)
X = dimensionless coordinate $= x/H$
y = coordinate (in long dimension of channel)
Y = dimensionless coordinate $= y/H$
z = coordinate (in downward direction with $\theta = 0$)
Z = dimensionless coordinate $= z/H$

Greek Letters

α = thermal diffusivity
β = volumetric coefficient of expansion with temperature
θ = angle of inclination of hot and cold surfaces from horizontal
ν = kinematic viscosity
τ = dimensionless time $= t\alpha/H^2$
ψ_i = i-component of dimensionless vector potential
$|\psi|$ = $\sqrt{\psi_x^2 + \psi_y^2 + \psi_z^2}$

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A Method of Predicting Diffusion Coefficients of Solutes at Infinite Dilution

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The prediction of the diffusion coefficient of solutes in solution has been the subject of numerous studies and several equations which allow the coefficient to be estimated have been proposed (Reid et al., 1977). A recent report by Sridhar and Potter (1977) proposes two equations, one for liquid-liquid systems and another for gas-liquid systems.

A simpler relationship has been found between the limiting diffusion coefficient of the solute and the self-diffusion coefficient of the solvent, which is given by the symmetrical relationship

$$D^0_{21}(V_2^* - \bar{v}_2^0)^{1/2} = D_{11}(V_1^* - v_1)^{1/2} \qquad (1)$$

where D^0_{21} and D_{11} are the limiting diffusion coefficient of the solute at infinite dilution and the self-diffusion coefficient of the solvent, respectively, V_2^* and V_1^* are the volumes at the critical temperature for the solute and solvent, respectively, and $\bar{v}_2^0$ is the partial molar volume of the solute in solution and v_1 is the molar volume of the solvent. This equation is suitable for both liquid-liquid and gas-liquid systems.

THE DATA

The extensive data in the literature pertaining to diffusion coefficients as surveyed by others (Dullien, 1972; Hayduk and Buckley, 1972; Reid et al., 1977; Sridhar and Potter, 1977; and Van Greet and Adamson, 1964) was used to test Equation (1). The data used included those for a total of thirteen different solvents and 126 solutes. For the solvent, V^* values were taken from the literature when available or otherwise estimated using a method proposed by Fedors (1978) which is simpler to apply and yields results comparable to the method of Lydersen (1955). The corresponding viscosities and densities were taken from the original data sources. V^* values for the solutes were estimated as for the solvents. $\bar{v}_2^0$ for liquid and solid solutes are generally unavailable, and so the value was taken equal to the molar volume of pure solute (in the liquid state). For solutes which are crystalline in the pure state, the volume corresponding to the liquid state was estimated using the method of Fedors (1974). For solutes which are in the gaseous state, $\bar{v}_2^0$ values were taken from the compilation of Hildebrand and Scott (1950).

RESULTS AND DISCUSSION

Table 1 summarizes the results obtained to date. The first column lists the solvent and the second column the number of different solutes whose diffusion coefficient at infinite dilution was determined in each solvent. Column 3 contains the average value of $D^0_{21}(V_2^* - \bar{v}_2^0)^{1/2}$, while the next column lists the values of the self-diffusion coefficient for the solvent calculated from the diffusion coefficient of the solute via Equation (1). The last column lists the value of the self-diffusion coefficient of the solvent as obtained from direct experimental measurement. As may be seen, the agreement between the two sets of values is satisfactory.

Data for five solutes in both ethanol and butanol as solvents did not follow Equation (1). For these two solvents, the calculated diffusion coefficients for symmetrically shaped solutes were higher than the equation would predict. These anomalous data are tabulated in Table 2. In column 5 of the table, there is listed the values of D^0_{21} calculated on the straightforward applica-