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A Numerical Study of Transient Natural Convection of Water Near its Density Extremum

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Abstract:

This numerical (CFD) study investigates the transient natural convection of water near its density extremum within a vertical cylindrical geometry. A non-Boussinesq approach is employed and the results are compared to previous studies. Distilled water having initial temperature of 8 ºC is used as the medium, while the entire cavity is insulated. This experimental chamber is enclosed within another glass cylinder, and coolant fluid at a fixed temperature of 0 ºC is pumped continuously through the annular region between the cylinders. Results of cooling curve measurements and the flow patterns present good agreement. From the resulting numerical outputs, it is evident that the density inversion of water has a significant influence on the natural convection in the cavity.

1. Introduction

Although the earliest systematic observations of the unusual expansion of water prior to its expansion upon freezing were in the experiments carried out by a group of court scientists working in the Galilean Accademia del Cimento in Florence [1], Thomas Charles Hope (1766-1844) was the first to carry out experiments to demonstrate it using convective techniques [2]. Hope used data obtained to estimate a value of between 39.5 ºF and 40 ºF for the temperature at which water has its maximum density. This is equivalent to a value between 4.2 ºC and 4.4 ºC. Greenslade [3] performed a graphical analysis of Hope's data and carried out a replica experiment. When Hope's temperature measurements are plotted as a function of time, plateaux on the cooling curves, similar to those obtained in many following investigations [4-7], are obtained.

Cawley and McBride [8] referred to the De Paz et al [5] experimental apparatus and results to investigate the transient natural convection of water in the vicinity of the density maximum. The present study uses the Cawley and McBride [8] experimental results to investigate numerically the effect of water density extremum on the transient natural convection in vertical cylinder. In order to reduce the discrepancies between CFD and experimental results, a non-Boussinesq model is considered. Instead of a linear density response as a function of temperature, a third order polynomial density-temperature relationship is applied. In addition, the third order polynomial state equations of specific heat capacity, c_p, thermal conductivity, k, and dynamic viscosity, μ, of water are incorporated. Also, an unsteady temperature as a function of time boundary condition on the cylinder sidewall provides a more realistic condition compared to a constant temperature boundary condition applied in previous work [8].

2. Methodology

The commercial CFD code FLUENT had been used to analyse the model flow characteristics and the results were compared with the published experimental data of Cawley and McBride [8]. In this numerical study a vertical glass cylinder of thickness 2.6 mm, inner diameter of 50.8 mm and height of

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128 mm as shown in fig. 1 was considered. Distilled water having initial temperature of 8 ºC was used as the medium, while the entire cavity was insulated. This experimental chamber was enclosed within another glass cylinder of diameter 103.4 mm, and coolant fluid at a fixed temperature of 0 ºC was pumped continuously through the annular region between the cylinders. The comparisons of cooling curves with [8] were made at three different vertical heights of 32, 64 mm and 96 mm as shown in fig. 1.

The finite volume method had been used to analyse the above flow characteristics by solving the governing equations for fluid flow and heat transfer (equations 1 to 3). The upwind differencing scheme was applied in discretising the convection-diffusion equations. The SIMPLEC (SIMPLE-Consistent) algorithm was then applied to solve the pressure-velocity coupling algorithms.

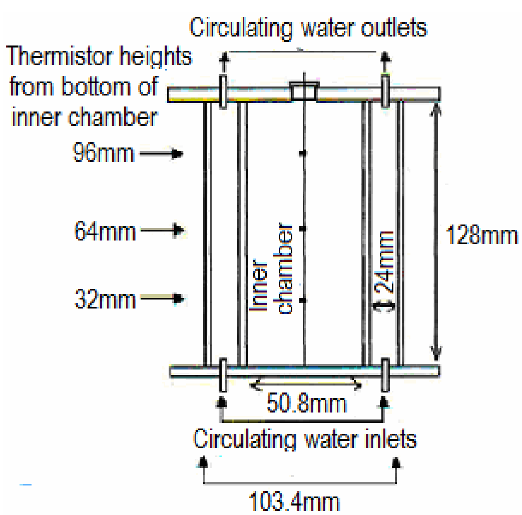

Fig. 1. Schematic diagram of the test cell.

2.1 State and governing equations

For the simulation purpose, the following equations in cylindrical coordinate form have been solved numerically for a Newtonian, incompressible fluid:

Continuity equation:

$$\frac{1}{r}\frac{\partial(ru)}{\partial r}+\frac{\partial w}{\partial z}=0 \qquad (1)$$

Momentum equations:

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+w\frac{\partial u}{\partial z}\right)=-\frac{\partial p}{\partial r}+\mu\left(\frac{\partial^2 u}{\partial r^2}+\frac{1}{z}\frac{\partial u}{\partial z}+\frac{\partial^2 u}{\partial z^2}\right) \qquad (2)$$

$$\rho\left(\frac{\partial u}{\partial t}+u\frac{\partial u}{\partial r}+w\frac{\partial w}{\partial z}\right)=-\frac{\partial p}{\partial z}+\mu\left(\frac{\partial^2 w}{\partial r^2}+\frac{1}{z}\frac{\partial w}{\partial z}-\frac{w}{z^2}+\frac{\partial^2 w}{\partial z^2}\right)-\rho g \qquad (3)$$

Temperature energy equation:

$$\rho c_p\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial r}+w\frac{\partial T}{\partial z}\right)=k\left(\frac{\partial^2 T}{\partial r^2}+\frac{\partial^2 T}{\partial z^2}\right) \qquad (4)$$

Convection in water, behaves in complicated manner when the temperature domain encompasses the 4 ºC, point at which the density of water reaches a maximum value of 999.9720 kg/m^3 at a pressure of one atmosphere. Therefore, in this work a non-Boussinesq approach was considered. Instead of a linear density response as a function of temperature, a third order polynomial density-temperature relationship was applied, which was tabulated in table 1. This polynomial was obtained from a graph plotted for data of water density between 0 °C to 20 °C [9]. In addition, polynomial thermophysical relationships for the specific heat capacity, c_p, thermal conductivity, k, and dynamic viscosity, μ, of water as tabulated in table 1 were incorporated [9].

Table 1 Thermophysical properties of water.

Property	Value of the property
ρ [kg/m^3]	9.3456e-2+8.660272T -2.3437e-2T^2+1.878703e-5T^3
c_p [J/kgK]	4.336773e+4-3.931164e+2T +1.31672T^2-1.472514e-3T^3
k [W/mK]	3.627368-3.691288T +1.400436T^2-1.6842e-7T^3
μ [kg/ms]	5.118959e-1-5.078044e-3T+1.689541e-5T^2 -1.882334e-8T^3

Comparison of predicted results with experimental data from [10] shows that it is necessary to incorporate all of the property-temperature relationships into the numerical model in order to achieve realistic results.

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2.2 Initial and boundary conditions

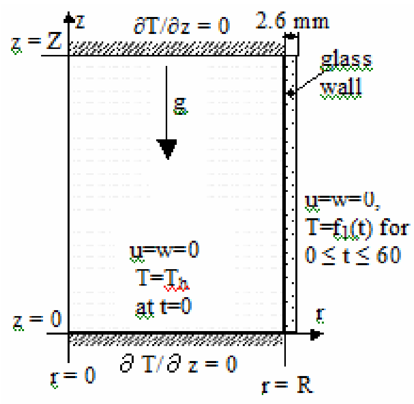

Fig. 2. Flow configuration.

As presented in fig. 2 the initial and boundary conditions were:

$$u = w = 0 \text{ and } T = T_h \text{ for } t \le 0 \quad (5)$$

$$T = f_1(t) \text{ at } r = R \text{ for } 0 \le z \le Z \text{ and } 0 \le t \le 60 \quad (6)$$

$$T = f_2(t) \text{ at } r = R \text{ for } 0 \le z \le Z \text{ and } 60 < t \le 960 \quad (7)$$

$$\frac{\partial T}{\partial z} = 0 \text{ at } z = 0 \text{ and } Z \text{ for } 0 \le r \le R \quad (8)$$

where

$$f_1(t) = -5e-05t^3 + 4.34e-02t^2 - 1.2274e+01t + 1.4357e+03 \quad (9)$$

$$f_2(t) = -2e-09t^3 + 6e-06t^2 - 7.0e - 03t + 2.7513e+02 \quad (10)$$

Cawley and McBride [8], in their publication used a constant temperature boundary condition of 0 ºC on the cylinder sidewall. The authors did claim that the temperature switchover in the annulus was not a true step. Therefore, it was clear that the true experimental boundary condition would not be isothermal. The present work applied polynomial temperature-time relationship to describe the temperature boundary condition on the wall concerned as presented in fig. 6(a). Curve in this figure was obtained using the experimental data [8] of the temperature in the annulus. This curve was presented by 2 third order polynomial equations 8 and 9. Results obtained verified that unsteady temperature wall condition produced improved results.

2.3 Sensitivity analyses

At the beginning of research, sensitivity studies were carried out in order to determine the grid and time step for the numerical solution. For the mesh analysis, grids of 100x40, 150x70 and 200x100 were chosen. The grid of 150x70 has been employed as it produced reasonable solutions. Four time steps were selected in order to access the sensitivity of temporal discretisation on the overall solution. These time steps were 6 s, 3 s, 1 s and 0.5 s and the results concluded that time step of 0.5 s did not produces much closer results compared to the experimental [8], hence a time step of 1 second was employed.

3. Results and discussions

Present numerical study simulates the transient convection of water within a vertical cylinder based on the experiments carried out by Cawley and McBride [8]. The effects of the water density anomaly on convection in water will be described.

Fig. 4 presents cooling curves for water in the experiment carried by Cawley and McBride [8] with the temperature being measured along the central axis of the cylinder at half the height of the cylinder. The cooling curve data present a departure from the exponential shape. A plateau or arrest that may be interpreted as being cause by a cessation of convective cooling in the centre of the cylinder can be seen. Fig. (4-5) present cooling curves for the three positions along the central axis of the cylinder, showing the variation of the plateau as a function of vertical position. These features will be understood when correlated with the results of flow visualization, later in this section.

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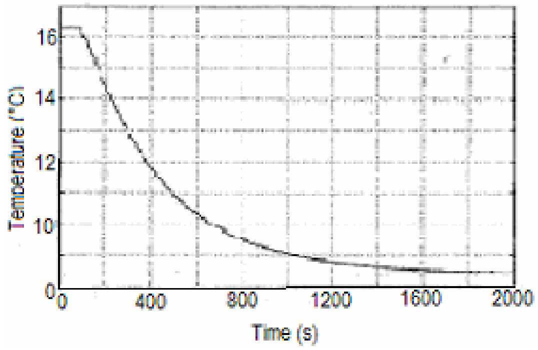

Fig. 3. Cooling curves for convection in water between 16 ºC and 8 ºC [8].

Cawley and McBride [8] simulated their experiment and present predicted cooling curves as shown in fig. 5. Although their experimental and numerical results demonstrate equal patterns, significant differences can be seen. The authors outline several causes for the discrepancies: the Boussinesq approximation approach that also assumes thermophysical properties of water (c_p, μ and k) to be constant; isothermal boundary condition of the cylinder wall; two-dimensional Cartesian model of the water layer. Present work tries to improve the numerical results by introducing a model considering these three factors, which are described in detail in the previous section. Fig. 4 highlighted that results closer to the experimental data [8] are obtained.

As verified in fig. (4-5), present work provides improved results compared to the previous study [8]. As a result of considering isothermal boundary layer on the cylinder wall in simulation, previous study [8] produced cooling curves starting with $T \approx 8$ ºC at $t = 0$. Experimental data [8] however, presents cooling curves with $T > 8$ ºC at $t = 0$, which are captured well in the present work. In addition, both experimental [8] and present work exhibit steady $T \approx 8.5$ ºC for approximately 70 s from the beginning of the experiment, which conclude that the cylinder wall does not reach 0 ºC spontaneously. Longer period is needed for the temperature at the axis of the cylinder to start decreasing, compared to as demonstrated in previous numerical work [8]. Furthermore, both experimental [8] and present work produce curves with greater cooling rates, as the curve for $y3$ = 96 cm is expected to be below 0 ºC after t = 1000 s as is evident in figure 4. In figure 5 however, this curve still does not go below 0 ºC at t = 1200 s. As will be described later, it is evident that the plateau temperature increases and the width of the plateau decreases as the probe height increases. This feature is well captured by both the experimental data [8] and the present work. The previous numerical study [8] however, demonstrates the plateau temperature for the upper probe ($y3$ = 96 cm) lower than the middle one.

Fig. 6(a-g) show the cooling curves and velocity quiver plots for the present numerical study of transient convection of water in the vicinity of density maximum. They indicate the following sequence of events as fully described in [8].

Table 3
Physical locations of lines A and B, and the corresponding times of measurements.

	Location of A (mm)	Location of B (mm)	Time (s)
CFD	113.5	82	390
PIV	106.2	76.3	340

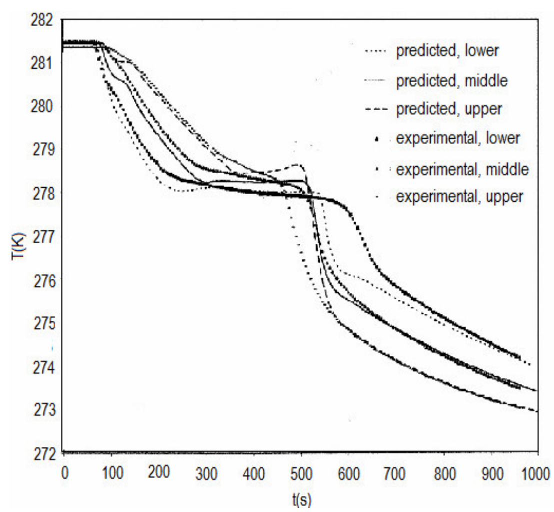

Fig. 4. Cooling curves comparing present numerical and experimental [8] results.

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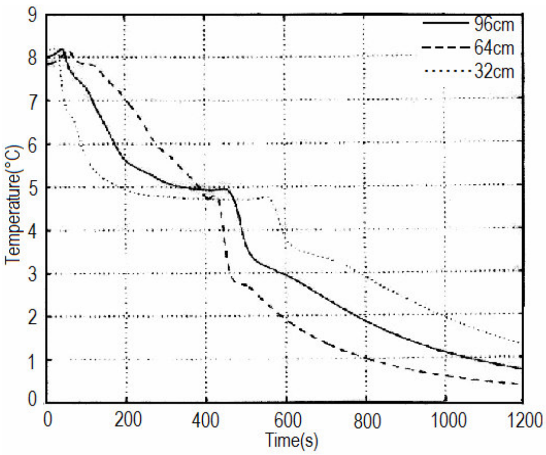

Fig. 5. Cooling curves [8].

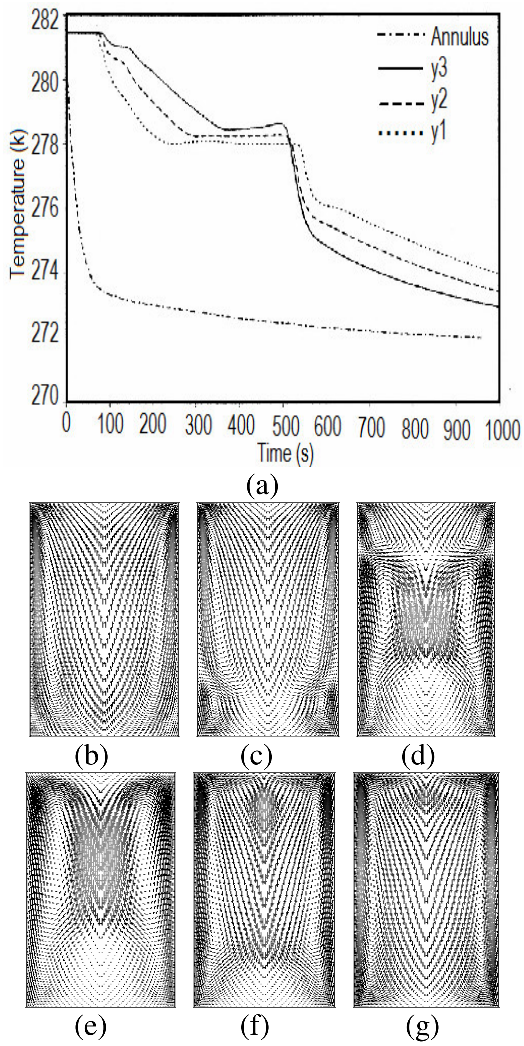

Fig. 6. (a) Cooling curves from simulation, (b)-(g) are velocity vector fields for the times of 160 s, 230 s, 390 s, 470 s, 560 s and 690 s respectively.

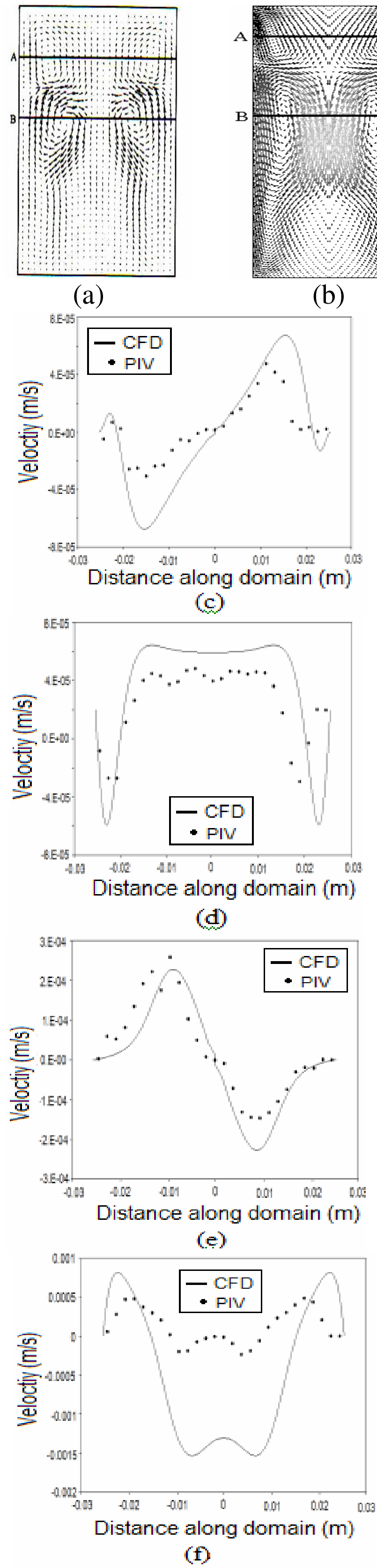

Fig. 7. Quantitative comparison of velocities.

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A study of the quantitative agreement between the experimental [8] and simulated results was also made. Fig. 7(a-b) show results from both cases for corresponding stages of flow evolution. The u and v components of the velocities were extracted for two different horizontal lines indicated on the diagram by 'A' and 'B'. Due to the uncertainties from the experimental data of Cawley and McBride as to the exact locations of A and B, they were chosen simply to pass through the centre of the vortices. Table 3 presents the physical locations of horizontal lines A and B for both predicted (CFD) and experimental data of Cawley and McBride (PIV).

In addition, the times for the measurement of velocity components on these lines were also tabulated. Fig. 7(c-d) compare the corresponding velocity values from both experiment and numerical. It can be seen that the quantitative agreement is good, with the data points from experiment and numerical showing the same features and being of the correct order.

4. Conclusions

A numerical analysis of natural convection in water in the vicinity of the density extremum has been carried out. The computational results show good concurrence with published experimental data. In order to capture the physics of such flows it was found necessary to incorporate thermodynamic and transport property-temperature relationships and activate higher order convection schemes in the numerical models. This, in conjunction with the use of a double-precision solver, helped produce numerical results that represented an amelioration on previously published computational data.

It is evident that there is a lack of high quality, quantitative experimental data in the current literature. This paucity of information makes it difficult to access accurately the effectiveness of new numerical approaches. The experimental area is one, which requires effort and resources to be directed to.

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