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 in enclosed spaces. Two cases are considered: flows in rectangular cavities; flows within a vertical cylindrical geometry. A non-Boussinesq approach is employed for both cases and the results are compared to previous studies. For the first case of rectangular cell, the cavity was not filled completely full of water, and a small gap is left at the top in order to have a free surface. Simulations are carried out with water having initial temperatures of 8, 12, 16 and 20 °C, which is equal to temperature of the opposing walls, while the entire cavity is insulated. The fluid is initially still and the temperature of one vertical wall is suddenly lowered to 0 °C. Measurements of the temperature distributions in the cavity were made at three different vertical positions: $y_1 = 0.01785$ m, $y_2 = 0.07545$ m and $y_3 = 0.1353$ m. Comparison of both predicted flow patterns and calculated temperatures to the previous study are presented, which confirms that good agreements are obtained. For the second case of vertical cylinder, distilled water having initial temperature of 8 °C 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 °C is pumped continuously through the annular region between the cylinders. The comparisons of cooling curves with previous work are made at three different vertical heights of 32, 64 and 96 mm. Results of cooling curve measurements and the flow patterns present good agreement. From the resulting numerical output of both cases, it is evident that the density inversion of water has a significant influence on the natural convection in the cavity.
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Nomenclature

Note: Units of temperature are context dependent.

\(a\) discretisation equation coefficients
\(A\) aspect ratio of the cylinder, \(Z/R\); cross-sectional area (m\(^2\))
\(b\) source term in discretisation equations (unit depend on \(\varnothing\))
\(c_p\) specific heat capacity (J/kgK)
\(d\) glass thickness (m)
\(D\) diffusion conductance; diameter (m)
\(F\) convective mass flux per unit area (kg/m\(^2\)s)
\(g\) acceleration due to gravity (m/s\(^2\))
\(h\) heat transfer convective coefficient (W/m\(^2\)K)
\(H\) height of liquid in cavity (m)
\(k\) thermal conductivity (W/mK)
\(L\) length of cavity (m)
\(Nu_D\) Nusselt number
\(p\) pressure (N/m\(^2\))
\(Pr\) Prandtl number
\(q\) heat flux (W/m\(^2\))
\(\dot{Q}\) volume flowrate (m\(^3\)/s)
\(r, \Theta, z\) cylindrical polar coordinates (m,rad,m)
\(R\) radius of cylinder (m)
\(Ra\) Rayleigh number
\(Re_D\) Reynold number
\(t\) time (s)
\(T\) temperature (K)
\(u,v,w\) component of velocity vector (m/s)
\(u\) velocity vector
\(\bar{u}\) mean velocity (m/s)
\(x,y\) Cartesian coordinates (m)
\(X\) dimensionless horizontal coordinate
\(Y\) dimensionless vertical coordinate
$Z$  
height of cylinder (m)

**Greek symbols**

$\theta$  
dimensionless temperature

$\mu$  
dynamic viscosity (kg/ms)

$\nu$  
kinematics viscosity ($m^2/s$)

$\rho$  
mass density ($kg/m^3$)

$\gamma$  
density inversion factor

$\varnothing$  
general property (units depend on property)

**Subscripts**

c  
cold

e,w  
east and west face values

$E, W$  
east and west nodal point values

$h$  
hot

$i$  
inside

$I, i$  
horizontal direction of staggered grids

$J, j$  
vertical direction of staggered grids

$\text{max}$  
maximum

$\text{nb}$  
neighbour cells

$o$  
outside

$p$  
nodal value

**Superscripts**

$*$  
guessed value

$'$  
corrected value
Chapter 1

Introduction
1.1 Introduction

The basic mechanisms of fluid flow and heat transport in natural convection arising from temperature differences alone have been well-established [1], [2] and [3]. It has been extensively studied in the past because of its importance to both engineering applications and the controlling mechanism in many naturally occurring processes such as meteorology, geophysics, astrophysics, nuclear reactor systems, solar energy systems, energy storage and conservation, fire control, food, and metallurgical industries.

Although natural convection heat transfer coefficients are relatively small, many devices depend largely on this mode of heat transfer for cooling. In the electrical engineering field, transmission lines, transformer, rectifiers, electronic devices, and electrically heated wires such as the heating elements of an electric furnace are cooled in part by natural convection. This has led to a large number of investigations on the subject that have been undertaken over recent years. A current example is the investigation carried out by Ganan et al. [4] in order to obtain higher thermodynamic cycles for the Spanish thermo electric plants, Almaraz Nuclear Plant. Since the artificial dam, Lake Arrocampo, is an open system consisting of thermal screens, it is strongly influenced by the weather conditions existing in the environment. This may lead to a power limitation during the summer due to the vacuum losses in the condenser. Therefore, a technical evaluation of the feasibility of introducing water cooling towers in parallel with the present cooling system has been carried out.

The technical developments in the computer and telecommunication industries also have created an impact on the natural convection heat transfer discipline. Transient behavior can be initiated at the system start-up or shut down. During these events, heat flux change with time, lead to temperature changes that may affect the system performance. Thus there is a need to investigate the transient thermal behavior of the system. Many researches are focused on this area including Incropera [5] and Bhowmik and Tou [6]. The studies verify that natural convection offers more reliable, low cost and maintenance free electronic cooling. As the circuit densities on the equipment increase the difficulty to rely on air-cooling. It is found
that water appears to be the most appropriate coolant in direct immersion cooling, as it has large specific heat and high thermal conductivity [7].

Investigations on natural convection also play a significant role in food processing applications. For instance in the conventional canning processes that extend the shelf life of food products and make the food safe for human consumption by destroying the pathogenic microorganisms. The sterilization of the canned food is usually carried out by steam heating to a temperature sufficient to kill the microorganisms. The time required for the sterilization process depends on the product specifications, container type and size, and its orientation, as well as the heating medium characteristics. Excessive heating will affect food quality and its nutritional properties. Although most existing mathematical analyses are for conduction heated products, due to the simplicity of the analytical and numerical solutions, detailed analysis of the convection heating, usually using water to simulate liquid food, is of great importance in the food industry [8] and [9]. Therefore, estimation of the heat transfer rates is essential in order to obtain optimum processing conditions and to improve product quality. Also, a better understanding of the mechanism of the heating process will lead to an improved performance in the process and may lead to some energy savings.

Extensive literature on the natural convection of near shore lake waters, reservoir sidearm or other shallow water bodies with a sloping bottom suggest its great importance in the environmental field [10], [11] and [12]. A recent example is the study carried out by Lei and Patterson [13] in order to understand the heat transfer and exchange of nutrients or pollutants from the coastal region to the interior waters of lakes and reservoirs. The heating and cooling through the water surface form a complete diurnal forcing cycle, to which real lakes and reservoirs are always subjected.

The great majority of previous studies on natural convection have been performed under the Boussinesq fluid approximation, which stipulates a linear relationship between density and temperature. However water, the most abundant liquid on earth, exhibits an extremum in the density-temperature relationship at about 4 °C. This nonlinear behaviour, termed the density inversion, brings forth a major dynamic ingredient to natural convection.
This phenomenon has important implications on engineering applications. In beverage storage tanks for example, it is often required that the contained fluid should be maintained at a low temperature near the freezing point. Cool-down of a liquid from the initial state high temperature to a target temperature is a crucial mission in this system. A key element is to predict the time scale for the fluid to reach a desired temperature level. These are based upon a proper understanding of the time-dependent structures of flow and temperature fields, as the system encompasses the density inversion effects during its course of cool-down [14].

In addition, information about the variation of the temperature corresponding to the density maximum is of particular interest to oceanographers. Natural convection in the oceans is driven not only by temperature-induced density variations, but also by density gradients generated by differences in salt concentration, so-called double-diffusive convection.

1.2 Literature Review

Natural convection in enclosed spaces of various forms occupies a large portion of the heat transfer literature, reflecting the significant number of investigations on the subject that have been undertaken over the years. In the vast majority cases, flows in rectangular cavities and within a vertical cylindrical geometry have been considered. Both cylindrical and rectangular geometries will be addressed in the present work. Most of previous studies are concerned with fluids for which Boussinesq approximation that assumes all properties of the fluid, except linear density-temperature relationship in one term to be constant and not to vary with temperature. Convection in cold water, however, behaves in complicated manner when the temperature domain encompasses the 4 °C, point at which the density of water reaches a maximum value of 999.9720 kg/m³ at a pressure of one atmosphere. In general, other fluids such as gallium, tellurium, antimony and molten bismuth posses a density extremum in the density-temperature relationship. However, among those fluids water, one of the common fluids occurring in nature, is the most important. Therefore, the main objective of this study is the investigation of the macroscopic
effects of the water density maximum on transient natural convective flows in pure water at temperatures in the vicinity of the density maximum.

1.2.1 Rectangular cavity

While many numerical studies have been reported in the literature concerning the steady-state convective flow in a variety of cavities having different types of boundary conditions, the transient natural convection condition is of interest in the present work. All of the investigations revealed that the flow structure and the heat transfer are strongly influenced by the density inversion. Robillard and Vasseur [15] and [16] described numerical simulations of transient natural convective cooling in two-dimensional rectangular enclosures with all walls being isothermal, at temperatures including the density maximum. The streamline patterns presented include all the essential features: initial double cell flow pattern, formation of an extra convection cell and ultimate reversal of the flow. As well as studying the streamline and temperature contour information, a study of heat transfer was also made. The authors conclude that the overall rate of heat loss from the sample is less in the case where the density anomaly is involved compared to a simulation where the density anomaly is not present.

A number of experimental studies which were concerned with transient natural convection flow of water in a temperature range where the density inversion of water is present have been published. Inaba and Fukuda [17] investigated natural convection flow in an inclined rectangular cavity where the temperature of one wall was maintained at 0 °C, while the temperature of the opposite hot wall was varied from 2 to 20 °C. Lankford and Bejan [18] conducted experiments in a vertical enclosure where a constant heat flux boundary condition was imposed on the hot vertical wall, while the opposite wall was cooled. A combined experimental and analytical investigation of two-dimensional natural convection in a rectangular cavity was reported by Seki et al. [19]. The cold vertical wall was kept at 0 °C, while the temperature of the hot wall was varied from 1 to 12 °C. The predicted and measured temperature profiles had the same trends, but the agreement was not satisfactory.
Braga and Viskanta [20] reported an experimental and theoretical investigation of transient natural convective heat transfer to water near its maximum density in a 300×150×75 mm rectangular cavity. The experimental chamber was never fully filled with water, but rather had a gap of about 3 mm at the top. This specified a free-slip boundary condition for the top boundary in their simulations with all other boundaries having the no-slip boundary condition. Initially, water inside the cell was at a uniform temperature, and then the temperature of one of the cold vertical walls was suddenly lowered and kept at 0 °C. The hot wall was maintained at a constant temperature during the course of each experiment and was equal to the initial temperature of the water that varies from 8 to 20 °C. Solutions of the governing equations were obtained numerically for all experiments performed. Long exposure streamline photographs for flow visualization and predictions of the flow patterns as well as a comparison of measured and calculated temperatures were presented. Given that all of their experiments encompassed the density maximum, two counter rotating convective cells were evident in their simulations. The expected symmetric double cell flow corresponding to hot and cold boundary condition respectively was not produced. According to the authors, asymmetric flow is a consequence of the combination free-slip and no-slip wall boundary conditions. When comparing their experimental and numerical results, the authors note that the temperature invariance of various properties of water in their simulations (with the exception of water density in the body force term of the momentum equations) is a limiting factor in terms of the agreement between the two sets of results. The present work uses Braga and Viskanta [20] experiments and numerical boundary conditions to simulate the transient natural convection in rectangular cavity which is presented in the first part of the study. However, a non-Boussinesq model is considered, where thermo physical properties of water vary as a function of temperature, in the manner of the CFD work by Scanlon and Stickland [21].

McDonough and Faghri [22] presented both experimental results and numerical simulations of transient and steady state convection in a 160×120×120 mm rectangular enclosure with the side walls held at different temperatures which encompass the density maximum. In conducting their experiments, the initial fluid temperature was maintained at either 5 °C or 8 °C while one of the side walls was
suddenly reduced to 0 °C. The flow patterns were visualized by a pH indicator technique and recorded on video. Quantitative velocity measurements were made by observing flow patterns and referencing a grid in the field of view. The authors observed the same asymmetrical flow patterns, and concluded that the symmetrical flow could not be obtained within a rectangular enclosure due to the shape and scale factors.

Tong and Koster [23] studied transient natural convection in a water layer subjected to density inversion numerically using the finite element method. The non-Boussinesq parabolic density-temperature relationship was incorporated. In the analyses of four-sided enclosures of different aspect ratios, the vertical walls were set to be isothermal with the horizontal walls set to be adiabatic. In each numerical simulation, one vertical wall was set to be 0 °C with the other being set to various values. The results illustrated that the temperature difference which determines the position of the maximum density plane in the water layer, can alter flow field and heat transfer substantially. The significant effect of aspect ratio on transient natural convection was also investigated. The heat transfer was maximized in a square enclosure and is less at other aspect ratios.

A more recent work carried out by Osorio et al.[24] investigated the transient natural convection of water near its density inversion in an inclined square cavity, both experimental and numerically. The simulation applied the spectral elements method. In the study, a square cavity with two adiabatic side vertical walls, filled with cold water in the density inversion range. The bottom surface of the cavity was heated from below at constant, uniform temperature, while the opposite top surface is kept at lower temperature. The cavity has an inclination angle with respect to the vertical direction. The results for the flow patterns, temperature distributions and average heat transfer coefficient agree well with numerical results reported in Lin and Nansteel [25]. They confirmed though, the inconsistencies of the experimental results of Inaba and Fukuda [17].
1.2.2 Vertical Cylinder

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 [26], Thomas Charles Hope (1766-1844) was the first to carry out experiments to demonstrate it using convective techniques [27]. Hope used data obtained to estimate a value of between 39.5 °F and 40 °F for the temperature at which water has its maximum density. This is equivalent to a value between 4.2 °C and 4.4 °C. Greenslade [28] 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 present transient simulation, are obtained.

De Paz et al. [29] published a paper describing an experiment (the same in all respects to that performed by the court scientists of the Accademia del Cimento in Florence) to demonstrate the density maximum phenomenon by effectively constructing a water-in-glass thermometer, with a water in a glass bulb attached to a capillary tube. In 1987 [30], they published the results of convection experiments which they carried out using a vertical cylinder of water. These experiments did not focus on the density anomaly, being carried out at temperatures in the range 6 °C to 21 °C. The resulting graphs of temperature versus time were approximately decaying exponential in form, displaying a point of inflection where the rate of cooling increases from the moment of initiation of the experiment and reaches a maximum rate of cooling. The rate of cooling begins to decrease after this point as the fluid temperature approaches that of the boundary. The analytical model was extended to include generic boundary conditions allowing boundary temperatures to be specified [31]. This was followed by a paper published in 1989 [32], whereby the model of convection was further extended to include fluids with density maxima. In their 1990 paper [33], the group returned to the experimental results. An apparatus is described which allows a cylinder containing the test fluid to have coolant at either of two fixed temperatures circulated about it. Results are presented from experiments where a sample of water, initially at equilibrium with the boundary at some temperature
greater than 4 °C, is cooled to a temperature less than 4 °C. These results show a
temperature profile where the usual approximate exponential decrease is modified by
a plateau appearing at the temperature somewhat above 4 °C. Results from a
warming experiment are also shown, giving rise to a plateau at a temperature
somewhat less that 4 °C. In 1993, the group published a short report comparing
experimental results of convection in water about 4 °C with their analytical model
[34]. A paper published in 1997 presented another comparison between experimental
and theoretical results [35]. The experimental results were obtained using an
improved version of the apparatus described in their 1990 publication. A model
convection based on that described in 1989 was used to obtain the theoretical results.

Kwak and Kuwahara [14] carried out a numerical study of transient natural
convective cool-down process of water in a cylindrical container, where a quadratic
function density-temperature relationship of water was incorporated. The authors
claimed that their study is motivated by the restricted Rayleigh numbers range in
previous studies. Therefore, the convection effect would not be prominent;
consequently, the time-dependent variations of the numerically-acquired Nusselt
number did not deviate much from the pure conduction solution. In addition, due to
the limited coverage of the relevant parameters, the effects of the Rayleigh number
and of the initial temperature (the density inversion factor) on the global cool down
process were not elucidated. In their study, calculations cover a much extended range
of values of Rayleigh number $Ra$, the aspect ratio $A$ and the density inversion factor
$\gamma$: $10^5 \leq Ra \leq 10^7$, $1.0 \leq A \leq 10.0$ and $0.0 \leq \gamma \leq 3.0$. The objective was to gain a
thorough basic understanding of the underlying physical phenomenon in the
convective cool down process encompassing the maximum density temperature. The
study considers a vertically-mounted cylindrical container which was completely
filled with water. Water was initially at rest and isothermal at a temperature greater
than temperature when maximum density occurs. The whole vertical side wall was
abruptly cooled to temperature less than maximum density temperature. The
horizontal walls were thermally insulated. Based on the structures of the side walls
boundary layer at early times, three characteristics flow regime were identified. The
qualitative early time behaviour was determined by the density inversion factor. The
intermediate-stage features for large density inversion factor disclosed the flow
restructuring. When the aspect ratio or Rayleigh number is large, boundary layer wave are monitored for moderate values of density inversion factor. The analysis of time-dependent heat transfer characteristics suggest that the cool down process is divided into several transient sections. They also estimated the relevant time scales for the overall cool-down process. Also elaborated are the specific effect of Rayleigh number, density inversion factor and the aspect ratio on each evolutionary stage.

Cawley and McBride [36] referred to the De Paz et al [33] experimental apparatus and results to investigate the transient natural convection of water in the vicinity of the density maximum. Results were presented both from cooling curve measurements and from flow visualization experiments (using particle image velocimetry), and a comparison was made with simulations. They showed a simple flow pattern at the early of experiment as the density state function is linear: fluid close to the boundary walls falls relative to the fluid in the interior of the cylinder, and this initiates a cyclical flow whereby boundary fluid descends and interior fluid rises, and there is a continual exchange until thermal equilibrium is reached. The reversal of the overall flow direction as the temperature crosses the maximum density region gives rise to a plateau feature in the cooling curve, which may be explained by the formation of the rising toroidal structure along the column boundary. This feature effectively diverts flow away from the inner region of the cylinder, resulting in the temporary cessation of convective cooling within this region. They also observed that the plateau occurs at different temperatures depending on the height of the temperature probe along the central axis: the plateau temperature increases and the width of the plateau decreases as the probe height increases. The present study uses the Cawley and McBride [36] experimental results to investigate numerically the effect of water density extremum on the transient natural convection in vertical cylinder, which is presented in the second part of the study. In order to reduce the discrepancies between CFD and experimental results, once again a non-Boussinesq model is considered. For the density 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, \( \mu \), of water are incorporated. Also, the governing equations expressed in cylindrical coordinates (rather than the Cartesian coordinates) are
introduced in the simulations, giving a more appropriate comparison with the PIV results. Finally, an unsteady temperature as a function of time boundary condition on the cylinder side wall provides a more realistic condition compared to a constant temperature boundary condition applied in previous work [36].
Chapter 2

Methodology
This chapter describes the numerical solution methodology in investigating the transient natural convection of water in enclosed spaces. Two cases are considered: section 2.1 analyses flows in rectangular cavities; section 2.2 considers flows within a vertical cylindrical geometry.

2.1 Rectangular Cavity

The commercial CFD code FLUENT has been used to analyse the model flow characteristics and the results were compared to the published experimental data of Braga and Viskanta [20]. The geometry considered was a two-dimensional water layer in a rectangular test cell having inside dimensions of 150 mm in height, 300 mm in length, and 75 mm in depth as shown schematically in Figure 2.1. The cavity was not filled completely full of water, and a small gap is left at the top in order to allow for thermal expansion. Simulations were carried out with water having initial temperatures of 8, 12, 16 and 20 °C, which was equal to temperature of the opposing walls, while the entire cavity was insulated. The fluid was initially still and the temperature of one vertical wall was suddenly lowered to 0 °C. Measurements of the temperature distributions in the cavity were made at three different vertical positions: \( y_1 = 0.01785 \text{ m}, \ y_2 = 0.07545 \text{ m} \) and \( y_3 = 0.1353 \text{ m} \), as shown in Figure 2.2. The non-linear dependency of density with temperature has been incorporated into the model and the outputs are shown in the next section.
Figure 2.1 Schematic diagram of the test cell in [20]: (a) front view; (b) end view.

Figure 2.2 Three different vertical positions of cavity specified for comparison purpose.
2.1.1 State and Governing Equations

For the simulation purpose, the following equations have been solved numerically for 2-D, incompressible, Newtonian fluid in Cartesian coordinates:

Continuity equation:
\[
\frac{\partial \rho}{\partial t} + \nabla . \rho \mathbf{u} = 0
\]  (2.1)

Momentum equation:
\[
\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla . (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla . (\mu \nabla \mathbf{u}) + \rho \mathbf{g}
\]  (2.2)

Temperature energy equation:
\[
\frac{\partial \rho c_p T}{\partial t} + \nabla . (\rho c_p \mathbf{u} T) = \nabla . (k \nabla T)
\]  (2.3)

Also, two dimensionless variables were introduced:
\[
X = \frac{x}{L}, \theta = \frac{T - T_c}{T_h - T_c}
\]  (2.4)

Most of previous studies [15-20] were concerned with fluids for which Boussinesq approximation was employed to simplify the equations. In fluid dynamics, the Boussinesq approximation is used in the field of buoyancy-driven flow. It states that density differences are sufficiently small to be neglected, except where they appear in terms multiplied by \( g \), the acceleration due to gravity. The essence of the Boussinesq approximation is that the difference in inertia is negligible but gravity is sufficiently strong to make the specific weight different between the two fluids. Therefore in most natural convection analyses, the density was assumed to be constant and not to vary with temperature except in the buoyancy term of the Navier-Stokes equation. The linear density response as a function of temperature is as follow:

\[
\rho = \rho_o (1 - \alpha (T - T_o))
\]  (2.5)

where \( \rho_o \) and \( T_o \) indicate reference quantities.
Convection in water, however, behaves in complicated manner when the temperature domain encompasses the 4 °C, 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 2.1. This polynomial was obtained from a graph plotted for data of water density between 0 °C to 20 °C [37] as demonstrated in figure 2.3 (a). In addition, graphs in figures 2.3 (b) to (d) referring to [37] were plotted in order to obtain the third order polynomial state equations of specific heat capacity, $c_p$, thermal conductivity, $k$, and dynamic viscosity, $\mu$, of water as tabulated in table 2.1. Figure 2.4 shows that it is necessary to incorporate all of the property-temperature relationships into the numerical model in order to achieve realistic results.