Direct numerical simulation of mixed convection of a liquid metal in the vertical rectangular channel

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Abstract. In the present work, mixed convection was studied using the direct numerical simulation (DNS) method for the upward flow of a liquid metal (Pr = 0.025) in a vertical rectangular heated channel. The Reynolds number (Re) varied from $10^4$ to $2 \times 10^4$. The criterion for the appearance of thermogravitational convection, as well as the characteristic of the intensity of its influence, was the Grashof number (Gr), which varied in the range from 0 to $4 \times 10^9$. A significant and ambiguous effect of free convection on hydrodynamics and heat transfer, which depends on the ratio $Gr/Re^2$ and the Prandtl number, is obtained.

1. Introduction
In conditions of mixed convection, the processes of stimulated heat transfer are significantly complicated by the action of the buoyancy force. The degree of influence of thermogravitation depends directly on the combination of dimensionless parameters: Re, Gr, Pr; the nature of the impact changes also, in other words the influence predominates either on the turbulence field or on the time-averaged flow.

At the moment there are many numerical and experimental works devoted to this topic. However, the vast majority of studies were performed for liquids with a moderate Prandtl number (for example: water or air [5,7]). Works devoted to liquid metal are much less. Currently, there are some experimental works (e.g [7-10]), which mainly dealt with the flow in the pipes, as well as numerical studies in pipes and channels, conducted using turbulence models (e.g [11-13]).

In this paper, using the DNS, the viscous-inertial-gravitational regime of liquid metal (Pr = 0.025) and also the nonmetallic coolant-water (Pr = 4) was studied, which allowed us to compare the behavior of the two media, and verify the used CFD-code better.

2. Methods

2.1. Physical model and governing equations
The geometry of the flow is shown in figure 1. The upward flow of a viscous incompressible fluid with constant physical properties in a rectangular channel is considered. This case corresponds to a stable stratification \( g \frac{\partial \rho}{\partial x} > 0 \). The fluid moves under the action of an applied pressure gradient, the
walls of the channel are heated uniformly along the length and perimeter by the heat flux \( q \). The solution did not take into account the contribution of viscous dissipation and the work of pressure forces. The fully developed flow and heat transfer are considered.

The problem was solved in a dimensionless form in a Cartesian coordinate system \((X,Y,Z)\). The width of channel \( A \), average flow velocity \( U \) and time scale \( A/U \) were taken as the characteristic scales. The combinations \( qA/\lambda \) and \( \rho U^2 \) are used as the scales for the temperature and pressure. Here, \( \lambda \) and \( \rho \) are the thermal conductivity and density of the fluid.

![Figure 1. Geometry of the flow and the coordinate system. \( \vec{g} \) – gravity acceleration, \( q \) – uniform surface heating flux.](image)

The cross-section of the channel was a square \((H=A, -0.5 \leq Z \leq 0.5)\). The dimensionless length of the channel \( L \) was equal to 10. This domain length is sufficiently long to capture large scale structures without imposing a severe demand on the number of gridpoints in streamwise direction. The non-dimensional governing equations and the boundary conditions at the duct’s walls are:

\[
\nabla \cdot \vec{U} = 0, \quad (1)
\]

\[
\frac{\partial \vec{U}}{\partial t} + (\vec{U} \cdot \nabla)\vec{U} = -\nabla P - \nabla \bar{P} + \frac{1}{\text{Re}} \nabla^2 \vec{U} + \vec{F}_b, \quad (2)
\]

\[
\frac{\partial \theta}{\partial t} + (\vec{U} \cdot \nabla)\theta = \frac{1}{\text{Pe}} \nabla^2 \theta - U_x \frac{dT_{ws}}{dX}, \quad (3)
\]

\[
\vec{U} \bigg|_{Z=\pm0.5, \ Y=\pm0.5} = 0, \quad (4)
\]

\[
\frac{\partial \theta}{\partial Y} \bigg|_{Y=\pm0.5} = 1, \quad \frac{\partial \theta}{\partial Z} \bigg|_{Z=\pm0.5} = 1. \quad (5)
\]

The non-dimensional parameters are the Reynolds number \( \text{Re} \equiv A U \nu^{-1} \), Prandtl number \( \text{Pr} \equiv \nu \chi^{-1} \), and Grashof number \( \text{Gr} \equiv g \beta q A^4 (\lambda \nu^2)^{-1} \). The Peclet number \( \text{Pe} \equiv \text{Re} \cdot \text{Pr} \) is also used. Here, \( \nu, \beta, \) and \( \chi \) are the coefficients of kinematic viscosity, thermal expansion, and thermal diffusivity of the fluid, respectively.

Periodic boundary conditions are given at the input and output

\[
\vec{U}(X = L,Y,Z) = \vec{U}(X = 0,Y,Z), \quad (6)
\]

\[
\theta(X = L,Y,Z) = \theta(X = 0,Y,Z). \quad (7)
\]

The temperature field is represented as the sum
\[ \Theta(\vec{X}, t) = \left( T + \bar{T} \right) / (qA / \lambda) = \theta(\vec{X}, t) + T_m(X), \]  
(8)

where \( \theta \) is temperature fluctuations, \( T_m(X) = F^{-1} \int_U A dF \) is dimensionless mean mixed temperature, \( F \) is channel cross-sectional area, \( \bar{T} \) is mean mixed temperature.

Similarly, the pressure field is decomposed into an average component \( \bar{P}(X) \) with a constant gradient and pressure perturbations \( P(\vec{X}, t) \). The pressure perturbations are statistically homogeneous in the streamwise direction and satisfy the Poisson equation with periodic inlet and exit boundary conditions.

The buoyancy force induced by variations of temperature is determined via the Boussinesq approximation

\[ \vec{F}_b = -\frac{Gr}{Re^2} \cdot \theta(\vec{X}, t) \cdot \vec{e}_g \]  
(9)

\( \vec{e}_g \) is the unit vector in the direction of gravity.

The dimensionless mean-mixed temperature is known from the integral energy balance

\[ \frac{dT_m}{dX} = \frac{4}{Pe}. \]  
(10)

The Nusselt number is defined in our units as

\[ Nu = 1/\bar{\theta}_w, \]  
(11)

where \( \bar{\theta}_w \) is the temperature perturbation measured at the wall and averaged over the perimeter.

The friction coefficient is defined as

\[ f = -2 \frac{d\bar{P}}{dX}. \]  
(12)

2.2. Numerical model

The problem is solved using the second order finite-difference scheme described first as scheme B in [1] and extended to the flows with heat transfer and thermal convection in [2]. The spatial discretization scheme is of the second order and is highly conservative in the sense that, in the non-dissipative limit, it exactly conserves the mass, momentum and internal energy, while the kinetic energy is conserved with dissipative error of the third order. The conservation property is achieved as in [3], i.e., via discretization of the differential operators based on the velocity interpolated to the half-integer grid point (see [1, 2] for details).

The time discretization is of the second order. It uses the backward differentiation scheme with explicit two-layer extrapolation of the nonlinear and force terms. The thermal conduction and viscosity terms are treated implicitly. The standard projection method (see, e.g. [4]) is used to satisfy incompressibility.

The computational grid is structured with the points distributed uniformly in the \( X \)-direction and clustered toward the walls in the \( Y \)- and \( Z \)-direction both according to the coordinate transformation:

\[ Y = \frac{\tanh(C_y \varphi)}{2 \tanh(C_y)}, \]  
(13)

\[ Z = \frac{\tanh(C_z \varphi)}{2 \tanh(C_z)}. \]  
(14)
where $C_1$, $C_Z$ are coefficients determining the degree of clustering, and the grid is uniform in the transformed coordinate $-1 \leq \zeta, \psi \leq 1$.

The grid sizes and the values of $C_1$, $C_Z$ have been determined in the grid sensitivity studies to determine the grid that would allow us to capture accurately the flow’s behavior, while completing the simulations within reasonable time. Three grids were tested: 1) $N_x=128$, $N_y=96$, $N_z=96$, $C_y=C_Z=2$, $\Delta t=5 \times 10^{-4}$; 2) $N_x=192$, $N_y=128$, $N_z=128$, $C_y=C_Z=2$, $\Delta t=5 \times 10^{-4}$; 3) $N_x=192$, $N_y=256$, $N_z=256$, $C_y=C_Z=2$, $\Delta t=2 \times 10^{-4}$; where $N_x$, $N_y$, $N_z$ – the number of grid nodes in the $X$, $Y$, $Z$ direction respectively, $\Delta t$ – time step.

According to the criteria formulated for $0.006<Pr<7$ by Grotzbach for the channel flow [14], these numerical resolutions should be sufficient to allow a numerical simulation. The mean grid width $h$ which is required in a DNS for sufficient small scale resolution of the velocity field:

$$h \leq 6.26 \eta,$$  \hspace{2cm} (15)

where $\eta = \left( \frac{1.86}{\varepsilon} \right)^{1/4}$ is the Kolmogorov length and $\varepsilon$ is the local dissipation of the turbulence energy.

The corresponding local criterion for the DNS of the thermal field is:

$$h \leq 3.45 \eta, \hspace{2cm} (16)$$

where $\eta = \left( \frac{1}{\varepsilon} \right)^{1/4}$ is the Corrsin’s temperature microscale.

To approximate the dimensionless time-averaged dissipation $\varepsilon^*$ (variables are scaled to wall units by using the channel width $A$ and the shear velocity $u_\tau$) for forced flows near its maximum in the cross-stream profile, i.e. at the edge of the buffer layer at about $y^* = 30$, Grotzbach assumed local equilibrium between production and dissipation of kinetic energy and calculates the dissipation from the production by means of the Prandtl mixing length and by the logarithmic velocity profile:

$$\varepsilon^*(y) = \frac{1}{|0.4 y/A|}$$ \hspace{2cm} (17)

This gives a smallest Kolmogorov length $\eta^* = 1.86$. In our simulations the minimum of the grid width in $Y$- and $Z$-direction was $h_{\text{min}}^* = 0.37$ and the maximum $h_{\text{max}}^* = 5.11$ (this corresponds to the grid $N=3$ and $Re=10^4$).

The criteria for near-wall resolution need to resolve the viscous and the conductive sublayer of the mean velocity and respectively temperature field. We use a grid clustered toward the walls, thus this requirement is already covered by the small-scale resolution criterion.

3. Results

In a water flow, as the Grashof number increases, the profile of the time-averaged velocity tends to acquire an M-shape with the maximum value between the axis and the wall (figure 2). The subsequent increase in the thermal load reduces the maximum velocity value. Thus profiles lie lower than in the case of purely forced flow approaching the profiles characteristic of turbulent free convection along a vertical plane.

The deformation of the time-averaged velocity field in a liquid metal flow has a different character (figure 3). The distribution of the averaged velocity acquires an M-shape under the action of thermogravitational convection, which becomes more pronounced with increasing heat flux. The velocity gradient near the wall for large Grashof numbers and consequently the friction coefficient increase also.
Figure 2. The profiles of the time-average velocity in a water at $Re=10^4$: 1 – $Gr=0$, 2 – $Gr=3\cdot10^8$, 3 – $Gr=4\cdot10^8$, 4 – $Gr=6\cdot10^8$, 5 – $Gr=5\cdot10^8$, 6 – $Gr=1\cdot10^9$, 7 – $Gr=1\cdot10^9$, 8 – $Gr=4\cdot10^9$. Here and below we consider the cross-section $Y=0$.

The inhomogeneity of the time-averaged velocity field decreases with an increase in the Reynolds number (figure 4), which is associated with a decrease in the effect of thermogravitation.

Figure 3. The profiles of the time-average velocity in a liquid metal at $Re=10^4$: 1 – $Gr=0$, 2 – $Gr=5\cdot10^6$, 3 – $Gr=1\cdot10^7$, 4 – $Gr=1\cdot10^8$, 5 – $Gr=4\cdot10^8$.

Figure 4. The profiles of the time-average velocity in a liquid metal at $Re=2\cdot10^4$: 1 – $Gr=0$, 2 – $Gr=2\cdot10^7$, 3 – $Gr=5\cdot10^7$, 4 – $Gr=1\cdot10^8$, 5 – $Gr=4\cdot10^8$.

A qualitative change in the temperature profiles in a water flow (figure 5) and in a liquid metal flow (figure 6) is similar. The wall temperature increases at the initial stage of the effect of thermogravitation, the temperature profile becomes more elongated. The profile of the time-averaged temperature flattened appreciably with an increase in the Grashof number later, herewith the maximum temperature remained on the channel axis.

Figure 5. The profiles of time-averaged temperature in a water flow at $Re=10^4$: 1 – $Gr=0$, 2 – $Gr=3\cdot10^8$, 3 – $Gr=6\cdot10^8$, 4 – $Gr=40\cdot10^8$ ($\theta_w$ - wall temperature, $\theta_c$ - axis temperature).

Figure 6. The profiles of the time-average temperature in a liquid metal at $Re=10^4$: 1 – $Gr=0$, 2 – $Gr=2\cdot10^7$, 3 – $Gr=5\cdot10^7$, 4 – $Gr=1\cdot10^8$, 5 – $Gr=4\cdot10^8$. 
Thermogravitational effects entail a change in the friction coefficient and heat transfer coefficient. The Nusselt number decreases first in a water flow, reaches a certain minimum value and then again increases, significantly exceeding the value corresponding to purely forced flow (figure 7). A similar behavior is observed for the friction coefficient (figure 8).

**Figure 7.** The Nusselt number $Nu$ as a function of $\sqrt{E}$ in a water flow at $Re=10^4$ ($E=Gr/Pr/Re^4$): 1 – simulations; 2 – approximation [5].

**Figure 8.** The friction coefficient $\xi$ as a function of $\sqrt{E}$ in a water flow at $Re = 10^4$: 1 – simulations; 2 – approximation [5], 3 – experiments [6].

The picture obtained for a liquid metal flow is qualitatively similar to that observed in a water flow. However, the effect of thermogravitational convection is considerably less, and the effect of buoyancy force begins appearing at lower heat flux. The minimum Nusselt value becomes more pronounced with an increase in the Reynolds number and shifts to a zone of greater heating (figure 9, 10, 11).

**Figure 9.** The computed Nusselt number $Nu$ as a function of $Gr$ in a liquid metal flow at: 1 – $Re = 10^4$, 2 – $Re = 1.5 \cdot 10^4$, 3 – $Re = 2 \cdot 10^4$.

**Figure 10.** The Nusselt number $Nu$ as a function of $Gr/Re^2$ in a liquid metal flow at $Re = 2 \cdot 10^4$: 1 – simulations, 2 – experiments [7].

**Figure 11.** The computed friction coefficient $\xi$ as a function of $Gr$ in a liquid metal flow at: 1 – $Re = 10^4$, 2 – $Re = 1.5 \cdot 10^4$, 3 – $Re = 2 \cdot 10^4$. 
4. Conclusions
The stable stratification that occurs when the liquid flows upward in a vertical heated channel has a significant effect on the hydrodynamics and heat exchange of both non-metallic liquid and liquid metal. Heterogeneity of the density affects the average fields of velocity and temperature, which, in turn, leads to a change in the friction coefficient and the coefficient of heat transfer. The heat transfer deteriorates at the initial stage of the manifestation of thermogravitation, further increase in heating leads to an increase in the Nusselt number. A similar behavior is observed for the friction coefficient. The predominance of molecular heat transfer in a liquid metal decreases the relative influence of buoyancy force on heat transfer, but the behavior of the heat transfer coefficient coincides qualitatively with the dependence $Nu(Gr)$ observed in liquids with a moderate Prandtl number.

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