A 3D Low Mach Number model for high performance computations in natural or mixed convection newtonian liquid flows

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Abstract. Despite its widespread usage Boussinesq's approximation exhibits a domain of validity which is extremely restricted for liquids in terms of admissible temperature difference, less than 10 K for liquid water under standard atmospheric pressure. This strong limitation can be overcome for flows subjected to weak dynamical pressure by introducing thermal property dependence in the governing equations. This communication presents the dilatable model we have developed to perform 3D computations of natural or mixed convection of liquid water. It contains two main features: a formulation that casts the Newtonian fluid behaviour law in a Low-Mach-Number approximation along with an open boundary condition formulation. The difficulties related to the former stand in implementing a computationally efficient equation of state for water in the LMN approximation framework, whereas those related to the latter concern the treatment of Open Boundary Conditions in the projection algorithm used. Both Boussinesq's approximation and the proposed LMN models have been used to compute a mixed convection water flow in a horizontal channel uniformly heated from below at prescribed heat flux ($Re = 50$, $Ri = 3$), for which the steady state solution is characterized by longitudinal roll-like structures combined to localized thermal plumes. Both models coincide in the upstream part of the channel where the fluid temperature is low and then progressively differ further downstream as the local temperature increases. A very good agreement is obtained between the LMN computed flow structure and the experimentally observed one.

1. Introduction
The understanding of 3D natural or mixed convection flows can sometimes be essential in the optimization of industrial components (heat exchangers, mixers, etc.) or industrial processes for which one looks for an increase in global energetic efficiency. However, several difficulties have to be overcome in order to accurately compute these flows, more especially in the case of liquid flows subjected to temperature differences higher than few tens of Celsius degrees. Indeed, whenever they seem at first sight rather moderated these liquid temperature differences nevertheless lead to conditions far beyond the range of validity of the widely used Boussinesq’s approximation [1, 2]. The liquid water case is a particularly striking one since its admissible temperature range is less than 10 K under standard atmospheric pressure. This comes from the fact that in these conditions the density variation induced by the temperature difference generate a pressure gradient that can be several orders of magnitude greater than that of the dynamical pressure intrinsic to the flow. To overcome the Boussinesq’s approximation limitations in the
case of perfect gas the key strategy has been to introduce an acoustic filtering of the compressible Navier-Stokes equations along with the Low-Mach-Number assumption [3, 4, 5]. This kind of algorithms has also been successful to compute natural convection flows of supercritical fluids close to critical point [6]. On the other hand for the liquid cases and more especially liquid water flows, up to the authors best knowledge there is no Low Mach Number approximation that has been convincingly combined to any liquid equation of state.

Another major difficulty in computing mixed convection flows is raised as they are at least partially open flows, this means that one does not know a priori on which part of the boundary the flow either enters or gets out the computational domain. Moreover, in the present problem the set of governing equations are strongly non-linear, so the boundary conditions are necessarily local and approximated on the outflow boundary [7, 8, 9]. For the three-dimensional problems to be computed here the Navier-Stokes equations are parabolic so the hyperbolic types of outflow boundary conditions as suggested by Orlanski [10] no longer give satisfactory solutions.

In this communication a new Low Mach Number model is introduced to compute 3D natural or mixed convection water flows, beyond the Boussinesq’s approximation limit. Therefore, we have chosen to start back from a diphasic liquid-vapor Low Mach Number model [11, 12], from which we have introduced a liquid water equation of state [13], tailored to end up with a computationally efficient numerical algorithm. From this approach, it becomes possible to generalize the algorithm to other newtonian liquids, provided one can access to the thermal relationship between its thermal expansion coefficient and sound velocity. We have also adapted the resulting projection algorithm to account for open boundary conditions, in order to deal with the two supplementary internal variables related to the Low Mach Number approximation, namely the thermodynamic pressure and its temporal derivative. In order to compare their respective capabilities both classical Boussinesq’s approximation and the proposed LMN model have been used to compute a mixed convection water flow in a horizontal channel uniformly heated from below at prescribed heat flux (Re = 50, Ri = 3) in a configuration similar to that previously studied with the former model in [14].

2. Governing equations

The proposed model is based on the compressible Navier-Stokes equations under the Low Mach Number approximation, following only in part the standard approach from the pioneer works [3, 4, 5]. Unlike in the preceding works we do not specialize them to the perfect gas equation of state, just retaining the newtonian fluid form, and keeping at first a generic equation of state [11, 12]. Then we have introduced the involved thermo-physical properties of water (density, dynamical viscosity, thermal conductivity, sound speed, etc.), along with their thermal dependance.

2.1. A dilatable model for liquid water

We are interested in modelling natural or mixed convection of liquid water, for temperature difference of several tens of degrees Celsius and under moderated pressure conditions (from atmospheric pressure up to few bars). In these conditions, the compressible Navier-Stokes equations read in a non dimensional form [11]:

\[ \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{V}) = 0 \]  \hspace{1cm} (1)
\[ \rho \left( \frac{\partial \vec{V}}{\partial t} + \vec{V} \cdot \nabla \vec{V} \right) = -\frac{1}{Ma^2} \nabla p - \frac{1}{Re} \nabla \cdot \bar{\tau} - \frac{\rho}{Fr^2} \vec{e}_z \]  \hspace{1cm} (2)
\[ \rho C_p \left( \frac{\partial T}{\partial t} + \vec{V} \cdot \nabla T \right) = \beta \alpha T \frac{Dp}{Dt} + \frac{1}{Re Pr} \nabla \cdot \bar{q} + \frac{Ma^2}{Re} \bar{\tau} : \nabla \vec{V} \]  \hspace{1cm} (3)
In these equations $\rho(T, p)$, $C_p$, $\alpha$, $\beta$, $\vec{V}$, $p$, $T$ and $t$ stand for density, specific heat coefficient, thermal expansion coefficient, a velocity vector, pressure, temperature and time, respectively. The four non dimensional numbers involved are: the Mach number ($Ma = V_{ref}/c$, $c$ is the sound speed in the liquid, defined as $c = 1/\sqrt{\frac{\partial p}{\partial p} - \frac{\alpha^2 T}{C_p}}$), the Reynolds number ($Re = \rho_{ref} V_{ref} L_{ref}/\mu_{ref}$), the Froude number ($Fr = V_{ref}/\sqrt{g L_{ref}}$), and the Prandtl number ($Pr = \mu_{ref}/C_p \kappa_{ref}$).

Concerning the constitutive relationships for water, it is a newtonian fluid and obeys the Fourier law. Its equation of state is at this stage kept as a generic relationship between density, temperature, and pressure: $\rho(T, p) = f(T)g(p)$ where $f(T)$ and $g(p)$ are two functions (the first depends on temperature only, the second on pressure only), $\mu(T)$ and $k(T)$ are dynamic viscosity and thermal conductivity (both depend on temperature), respectively. The $f(T)$ function is derived from the thermodynamic definition of the volumetric expansion coefficient: $\alpha(T) = \frac{1}{\rho} \frac{\partial \rho}{\partial T} = -f'(T)/f(T)$. Furthermore, as $\alpha(T)$ is continuous and integrable over the temperature range of interest $[10 - 95^\circ C]$, integrating it enables to get the $f(T)$ expression, which reads: $f(T) = \exp(-\int_{T_1}^{T_2} \alpha(T)dT + \gamma e)$.

This set of governing equations (1), (2), (3), (4) is complemented by boundary and initial conditions, to be detailed later on.

### 2.2. A dilatable model for liquid water in the Low Mach Number limit

The Low Mach Number approximation of the governing equations is obtained in a classical way [3, 4, 5], by first expanding of all the variables ($U = \rho$, $\vec{V}$, $p$, $T$) with respect of the Mach number, as follows:

$$U(\vec{x}, t, Ma^2) = U_0(\vec{x}, t) + U_1(\vec{x}, t)Ma^2 + O(Ma^4)$$  \hspace{1cm} (5)

and then inserting these asymptotic expansions in the governing equations (1), (2), (3), (4). Recalling that $Ma << 1$, one obtains at zero order: $\vec{\nabla} p_0 = 0$, so $p_0(\vec{x}, t) = p_0(t)$ and $p(\vec{x}, t) = p_0(t) + p_1(\vec{x}, t)$. Then at first order one gets:

$$\rho_1 = f(T_1)p_0(t)$$  \hspace{1cm} (6)

$$\frac{\partial \rho_1}{\partial t} + \vec{\nabla} \cdot (\rho_1 \vec{V}_1) = 0$$  \hspace{1cm} (7)

$$\rho_1\left(\frac{\partial \vec{V}_1}{\partial t} + \vec{V}_1 \cdot \nabla \vec{V}_1\right) = -\vec{\nabla} p_1 - \frac{1}{Re} \vec{\nabla} \cdot (\mu(T_1)) \left[\nabla \vec{V}_1 + (\nabla \vec{V}_1)^T - \frac{2}{3} (\vec{\nabla} \cdot \vec{V}_1) I\right] - \frac{\rho_1}{Re Pr} \vec{c}_T^2$$  \hspace{1cm} (8)

$$\rho_1 C_p \left(\frac{\partial T_1}{\partial t} + \vec{V}_1 \cdot \nabla T_1\right) = \beta(T_1)\alpha(T_1)T_1 \frac{dp_0}{dt} + \frac{1}{Re Pr} \vec{\nabla} \cdot (-k(T_1) \nabla T_1)$$  \hspace{1cm} (9)

Two internal unknowns have appeared in this low Mach number approximation, namely the thermodynamic pressure ($p_0(t)$) and its time derivative ($dp_0(t)/dt$), so one has to provide two additional equations to determine them. The first one can be obtained by inserting (6) into (7), integrating by parts the second term and dropping the order one subscript, then it reads:

$$\frac{\partial}{\partial t} \left(p_0(t) \int_{\Omega} f(T) dv \right) + p_0(t) \int_{\partial \Omega} f(T) \vec{V} \cdot \vec{n} ds = 0$$  \hspace{1cm} (10)
The second extra equation can be obtained by combining (7), (9), (6) and the total differential of the density \( dp = \partial \rho / \partial \rho \, dp + \partial \rho / \partial T \, dT \), to obtain:

\[
\frac{dp_0(t)}{dt} = \frac{1}{\Omega} \left[ \frac{1}{RePrC_p} \int_{\Omega} c^2(T)\alpha(T) \vec{n} \cdot (-k(T)\vec{n}T) \, dv - p_0(t) \int_{\Omega} c^2(T)f(T)\vec{n} \cdot \vec{V} \, dv \right]
\]  

(11)

3. Numerical model

The above governing equations under the low Mach number approximation are dealt with a projection algorithm, adapted from that originally designed for incompressible and isothermal flows [16], later on extended to thermal flows and open boundary conditions [17]. The basic idea to deal with open boundary condition is to split the first order pressure in two terms: \( p_1(\vec{x}, t) = P_{LMN}(\vec{x}, t) + P_{OBC}(\vec{x}, t) \). The first term satisfies the following domain equation and boundary conditions:

\[
\Delta P_{LMN}(\vec{x}, t) = - \left[ \vec{n} \cdot \vec{V} + \frac{1}{\tau(T)p_0(t)} \left( \frac{1}{c^2(T)} \frac{dp_0(t)}{dt} - \frac{\alpha(T)}{RePrC_p} \vec{n} \cdot (-k(T)\vec{n}T) \right) \right] \quad \text{in} \ \Omega
\]

\[
P_{LMN}(\vec{x}, t) = 0 \quad \text{on} \ \partial \Omega_{OBC}
\]

\[
\frac{\partial P_{LMN}(\vec{x}, t)}{\partial n} = 0 \quad \text{on} \ \partial \Omega_{V}
\]

(12)

And the second term satisfies the following domain equation and boundary conditions:

\[
\Delta P_{OBC}(\vec{x}, t) = 0 \quad \text{in} \ \Omega
\]

\[
P_{OBC}(\vec{x}, t) = \frac{\alpha(T)}{Re} \vec{n} \left[ \nabla \vec{V} + (\nabla \vec{V})^T - \frac{2}{3} (\vec{n} \cdot \vec{V}) I \right] \vec{n} \quad \text{on} \ \partial \Omega_{OBC}
\]

\[
\frac{\partial P_{OBC}(\vec{x}, t)}{\partial n} = 0 \quad \text{on} \ \partial \Omega_{V}
\]

(13)

In these expressions \( \partial \Omega_{OBC} \) and \( \partial \Omega_{V} \) designate the boundary subset associated to the Open Boundary Condition [18] and that where a Dirichlet boundary condition is imposed for the velocity field, respectively.

3.1. Solution algorithm

Owing to the strongly non linear and intricate variable dependance the developed numerical model is based on a segregated algorithm, for which one algebraic system is associated to each unknown field \( (T, \vec{V}, P_{LMN} \text{ and } P_{OBC}) \). On the other hand, the other unknowns \( (f(T), p_0(t) \text{ and } dp_0(t)/dt) \) are obtained by solving their associated scalar equation (local for \( f(T) \) and integral for the two others). The solution algorithm is unsteady and consists in starting from an initial solution and then looping over time steps, until the requested time integration or steady state if any is reached. It reads as follows:

- solve for \( dp_0/dt(t + \Delta t) \), eq. (11);
- solve for \( T(t + \Delta t) \), eq. (9);
- update all physical properties: \( \rho(T), \mu(T), k(T), \alpha(T), \beta(T), c(T) \);
- solve for \( \vec{V}(t + \Delta t) \), eq. (8);
- solve for \( p_0(t + \Delta t) \), eq. (10);
- solve for \( p_1(\vec{x}, t + \Delta t) \), eq. (12) and (13);

3.2. Spatial and temporal discretisations and HPC implementation

The spatial discretization related to field unknowns \( (T, \vec{V}, P_{LMN} \text{ and } P_{OBC}) \) is performed by a standard Bubnov-Galerkin Finite Element Method. The velocity vector and thermal fields have been discretized with piecewise quadratic approximations \( (Q2) \) in each space direction, using hexahedral \( H27 \) Lagrange finite elements. On the other hand, the hydrodynamic pressure
field ($p_1$) is discretized with piecewise linear approximations ($Q1$) in each space direction, using hexahedral $H8$ Lagrange finite elements.

As previously mentioned the set of governing equations is highly nonlinear. So in order to efficiently compute both transient and steady state solutions with the same solution algorithm we have used a second order implicit time integration scheme ($BDF2$), together with a second order time extrapolation of the intermediate quantities not yet updated at a given substep of the solution algorithm [19].

This numerical model has been implemented in the PETSc environment [20], which give us access to High Performance Computations on massively parallel supercomputers such as an IBM SP6 at IDRIS and SGI Altix at CINES. The algebraic systems to be solved at each time step of the solution algorithm are undertaken with the Bi-Conjugate Gradient Stabilized iterative solver, preconditioned with the Additive Schwartz Method, both methods been efficiently implemented in the PETSc library [20].

4. Mixed convection of water flow in a horizontal channel heated from below

The considered problem concerns a mixed convection water flow that develops in a horizontal channel heated from below at prescribed heat flux (cf. fig. 1). The channel extends in the streamwise direction with a longitudinal aspect ratio $A = L/h = 75$ and has a rectangular cross section of spanwise aspect ratio $B = l/h = 10$. The prescribed heat flux is applied downstream an adiabatic entrance $A_e = L_e/h = 5$.

\[
\begin{align*}
\frac{\partial \theta}{\partial z} &= 0, \\
\partial \theta / \partial z &= 0
\end{align*}
\]

Figure 1. Sketch of computational domain and imposed boundary conditions.

The boundary conditions of this problem read:

- an isothermal Poiseuille flow is imposed at the inlet ($x = -A_e$): $u = u_{Poise}(y, z)$, $v = w = \theta = 0$;
- Open Boundary Conditions are imposed at the outlet ($x = A - A_e$) [18, 16, 17];
- lower horizontal wall ($z = 0$): $u = v = w = 0$ and $\partial \theta / \partial z = 0$ for $-A_e \leq x < 0$ or $\partial \theta / \partial z = q$ for $0 \leq x \leq A - A_e$;
- upper horizontal wall ($z = 1$): $u = v = w = 0$ and $\partial \theta / \partial z = 0$;
- lateral walls ($y = 0$ and $y = B$): $u = v = w = 0$ and $\partial \theta / \partial y = 0$.

The control parameters of this mixed convection water flow are the Reynolds number ($Re = \rho_0 \bar{u}_0 h / \mu_0 = 50$, with $\rho_0 = \rho(x = 0)$, $\bar{u}_0 = u(x = 0)$ and $\mu_0 = \mu(x = 0)$), the Rayleigh number ($Ra = 1.5 \times 10^4$, built on the imposed heat flux) and the water Prandtl number ($Pr = 6.9$ at 25°C). Based on mesh sensitivity analysis previously made in a comparable configuration [14] the computational domain is made up with 750x200x20 $H27$ hexahedral finite elements.
uniformly distributed in the streamwise, spanwise and vertical directions. This mesh is built on 24,677,941 velocity and temperature nodes, and 3,169,971 pressure nodes. Despite being probably not optimal this mesh resolution gives nevertheless a satisfactory representation of both thermal and fluid flow boundary layers to compute representative fluid flow structures and patterns. For the given set of control parameters the fluid flow is steady and made up of convective structures aligned in the streamwise direction. A very good agreement can be observed in fig. 2 where both experimental and computed fluid flow structures are displayed side by side. We have also tried to see in this problem where and how do any modelling differences take place between the classical Boussinesq’s approximation and the present dilatable low Mach number one. Indeed, if one has a detailed look at the heated lower wall (see fig. 3), one can see that both model display common features in the upstream three-fourth of the channel. However, as going further downstream, more and more differences occur as the wall temperature become higher and higher. Therefore, this is where the two models behave differently, since all physical properties except density are taken as constant in the Boussinesq’s approximation, whereas they vary with temperature in the LMN model. In particular the dynamic viscosity is decreased by 30% over a temperature increase of 20°C. Therefore, thermal plumes take place more easily as buoyancy increases and viscosity decreases resulting in the more perturbed flow structure. A more quantitative comparison is also proposed in fig. 4(a-b) where spanwise non dimensional heated wall temperature profiles are drawn at three downstream locations ($x = 10; 40; 70$) with both Boussinesq’s and dilatable low Mach number approximations. Theses plots show that the thermal plumes are very sensitive to any temperature difference, and they induce a slightly modified heat transfer, whenever comparable on average. Indeed, we have plotted in fig. 4(c) the streamwise profile of the Nusselt number, averaged over the spanwise direction. It turns out that Boussinesq’s approximation and LMN model give a very comparable heat transfer in the establishing zone ($x < 22$) where the flow structure takes place. But, taking thermal dependant physical properties as done in the LMN model decreases thermal boundary layers, which results in significantly higher heat transfer compared to the Boussinesq’s approximation.

5. Conclusion
An original numerical model has been developed to compute 3D natural and mixed convection water flows. It is based on a dilatable model derived under the low Mach number approximation for any newtonian fluids. Nevertheless, we have specialized it with a computationally efficient
Figure 3. Computed thermal field at the lower wall: a) with Boussinesq’s approximation; b) with the present LMN model.

Figure 4. Computed spanwise non dimensional heated wall temperature profiles at $x = 10; 40; 70$: a) with Boussinesq’s approximation; b) with the present LMN model; Streamwise profile of the spanwise averaged Nusselt number.

The equation of state for liquids and especially water, which is new up to the authors best knowledge. Moreover, the second originality of this model is to account for Open Boundary Conditions so that the two internal variables, namely the thermodynamic pressure and its time derivative, are fully consistant with them. Finally, this model has been implemented in a high performance environment to take advantage of massively parallel computers we have access to.

In order to show the new model capabilities we have computed a mixed convection water flow in a horizontal channel uniformly heated from below at a prescribed heat flux. The comparison of the present model results to those obtained with the classical Boussinesq’s approximation reveals that the latter underestimates the global heat transfer as it overestimates the thermal and dynamical boundary layers with respect to those obtained with the thermally dependent low Mach number model.

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