Large eddy simulations of air flow in a vertical heated pipe using unstructured Cartesian grids with local refinement

V I Artemov, M V Makarov, K B Minko and G G Yankov

National Research University "Moscow Power Engineering Institute"
Russia, 111250 Moscow, Krasnokazarmennaya, 14.

Email: viartemov@yandex.ru

Abstract. This paper presents the results of modeling of fully developed turbulent gas flow in a uniform heated vertical tube by using the LES method and Smagorinski model. Unstructured Cartesian grids with local anisotropic refinement were used for modeling hydrodynamics and heat transfer in cylindrical pipes. Such meshes unlike structured meshes in cylindrical coordinates allow to construct more detailed meshes for the LES method. In addition, such meshes allow to simulate flows in channels of arbitrary cross-section. To verify the proposed methodology the results of direct numerical simulation of turbulent air flow in a vertical heated tube for forced and mixed convection were used. Thus, for upward flows the most interesting case with significant laminarization flow due to the buoyancy influence was studied.

1. Introduction
During the last decade in nuclear power engineering the problem of constructing nuclear power plants with supercritical pressure (SCP) coolants is intensely discussed [1]. Single-circuit plant layout with a nuclear reactor cooled by SCP water, delivery to a turbine of slightly activated steam of 25 MPa/540°C parameters, and steam reheating make it possible to reach a thermal efficiency that is close to that of the present-day steam-turbine power plants burning fossil fuels. Due to using pseudo phase transition heat (∼1400 kJ / kg) and pronounced reducing water flow rate through the reactor, the dimensions of the apparatus and the plant as a whole decrease and considerable gain in capital cost can be obtained. Therefore it is very important to use the numerical simulation of hydrodynamics and heat transfer to SCP water in the channels of the nuclear reactor in different operation conditions for safety substantiation at the stage of pre-design studies of new generation nuclear power plants. At present computer simulations of turbulent heat transfer in channels are used different approaches which based on: the Reynolds averaged Navier-Stokes equations (RANS), large-eddy simulation (LES), direct numerical simulation (DNS) of turbulence, and various hybrid methods (RANS+LES).

In most cases for practical purposes results obtained using RANS models are quite satisfactory. However, for liquids with highly variable properties (typical representatives of which are the SCP coolants) RANS models do not allow to obtain reliable data for the regimes with a strong deterioration of heat transfer. In this sense very revealing the work [2], in which 14 popular models for the turbulent viscosity was used for heat transfer simulations in upward flow of water in heated pipe with performance parameters corresponding to the experiment K. Yamagata [3]. Although there were no regimes with a strong deterioration of the heat transfer, 10 models have shown quite unsatisfactory
results, other models have led only to qualitative agreements.

The authors know only three works that used the methods of the DNS [4,5] and LES [6] with respect to the flow of SCP water in vertical heated channels. Authors [4,5] used a structural meshes. The numbers of cells were about 7·10^6 in [4] and 62·10^6 in [5]. Other parameters of the regimes were chosen identical. In both studies the Reynolds number at the inlet of the pipe was Re=5400, the length of the pipe was L/d=30. As follows from comparison of the results [4] and [5] for two regimes marked differences in wall temperature were observed. One of the reasons is significantly different number of cells. In [6] a version of the WALE subgrid viscosity was used and the circular tube was simulated by a rectangular channel, the number of grid cells was about 12·10^6, the Reynolds number at the inlet was 35000. The results of LES simulation [6], despite some controversies in the problem statement, allowed to make a conclusion about the possibility and efficiency of application of LES for simulation and detailed studies of the real turbulent flows with large Re number and large lengths of channels.

In this paper the results of the use LES method for unstructured Cartesian grids with local refinement, implemented in the in-house CFD code ANES are presented. To validate the proposed method the results [7] of direct numerical simulation of mixed convection in a heated pipe were used. In [8] the DNS data were used to verify 10 different two-parametric models of turbulence. Only k-ε Launder-Sharma model [9] allowed to satisfactorily describe the deterioration of heat transfer due buoyancy, and other popular models (including k-ω model of Wilcox [10] and the SST model of Menter [11]) gave unsatisfactory results. Since the buoyancy are one of the most important effect of the variability of the liquid properties, the comparison with DNS results can be a good test for the proposed methodology of simulation of turbulent flows with strongly varying properties of the liquids.

2. Mathematical model

2.1. Problem statement

It is considered fully developed upward flow in a vertical tube with the radius R and the length Lz, heated with a constant heat flux qw. The Boussinesq approximation is used for the description of buoyancy forces.

In this case it is possible to reduce the problem to the case with periodic boundary conditions in the flow direction (z1-axis in the Cartesian or cylindrical coordinate systems):

\[ p_i = p_{cicl} - \beta_p z_1, \quad t_i = t_{cicl} + t_m(0) + A_T z_1, \quad u_{cicl} = u, \]

\[ A_T = \frac{t_m(L_z) - t_m(0)}{L_z}, \quad \beta_p = -\frac{p_m(L_z) - p_m(0)}{L_z} \]

\[ t_m(z, \tau) = \frac{1}{u_m A_t} \int u_m t dA, \quad u_m(\tau) = \frac{1}{A_T} \int u_m dA, \quad p_m(\tau) = \frac{1}{A_T} \int pdA \]  

Here \( u_1 \) correspond to velocity vector, \( p_i \) to static pressure, \( t_i \) to temperature, \( t_m \) to bulk temperature at \( z_1=\text{const} \), \( A_t \) to cross-sectional area of the pipe, \( p_m \) to mean pressure, \( u_m \) to average air speed, \( L_z \) to dimensional length of the tube.

Variables \( p_{cicl}, u_{cicl} \) and \( t_{cicl} \) satisfy periodic boundary conditions along the \( z_1 \) axis:

\[ p_{cicl}(z_1 = 0) = p_{cicl}(z_1 = L_z), \quad t_{cicl}(z_1 = 0) = t_{cicl}(z_1 = L_z), \quad u_{cicl}(z_1 = 0) = u_{cicl}(z_1 = L_z) \]  

(3)

Parameter \( \beta_p \) is associated with an average speed of \( u_m \). When solving non-steady problems, one can use the following conditions: \( \beta_p = \text{const} \) or \( u_m = \text{const} \). In the present paper, as in [7] the condition of constant flow rate \( u_m = \text{const} \) was used.

Parameter \( A_T \) is related to the wall heat flux \( q_w \) (\( A_w \) - area of tube wall):

\[ A_T = \frac{q_w A_w}{\rho c u_m A_T L_z} \]

(4)
For boundary conditions (5), the following problem arises. In steady problems the temperature $t_{icl}$ can be determined up to a constant, the choice of which depends on the method of processing the results of calculation. In non-steady problem the temperature $t_{icl}$ is uniquely determined, however a constant is determined by initial distribution at $\tau = 0$. In this paper it was chosen the condition of equality to zero the average temperature in the volume of the computational domain ($V_d$):

$$t_{icl,V} = \frac{1}{V_d} \int_{V_d} t_{icl} dV = 0$$  \hspace{1cm} (6)$$

When using (4) condition (6) must be satisfied for all points of time $\tau > 0$. This property was used to control precision of unsteady solution.

2.2. Governing equations and solution algorithm

The simulation used three-dimensional non-steady equations of the LES [13], written in dimensionless form in the Cartesian coordinate system:

$$L' = R, \quad U' = u_m, \quad P' = \rho u_m^2, \quad \tau' = \frac{R}{u_m}, \quad T' = \frac{q_a R}{\lambda},$$

$$x = \frac{x}{L'}, \quad u = \frac{u}{U'}, \quad p = \frac{p_1 + \rho g z}{P'}, \quad T = \frac{t_1 - t_{m0}}{T'}$$

where $x_1, p_1, t_1$ and $u_1$ – dimension values.

We assume that the density $\rho$, kinematic viscosity $\nu$, conductivity $\lambda$, heat capacity at constant pressure $c_p$ and coefficient of thermal expansion $\beta_T$ of the gas are constants. The gravity force is opposite to the $z_1$-axis. In this case, the system of governing equations can be written as:

$$\text{div}(\mathbf{u}) = 0,$$

$$\frac{\partial \mathbf{u}}{\partial \tau} + \text{div} (\mathbf{uu}) - \frac{1}{\text{Re}} \nabla u = -\frac{\partial \rho}{\partial x} + \frac{\partial}{\partial x_k} \left( 2v_{sgs} S_{ik} \right),$$

$$\frac{\partial \mathbf{u}}{\partial \tau} + \text{div} (\mathbf{uu}) - \frac{1}{\text{Re}} \nabla u = -\frac{\partial \rho}{\partial y} + \frac{\partial}{\partial y_k} \left( 2v_{sgs} S_{ik} \right),$$

$$\frac{\partial \mathbf{u}}{\partial \tau} + \text{div} (\mathbf{uu}) - \frac{1}{\text{Re}} \nabla u = -\frac{\partial \rho}{\partial z} + \beta_T + \frac{Gr}{\text{Re}^2} T + \frac{\partial}{\partial z_k} \left( 2v_{sgs} S_{ik} \right),$$

$$\frac{\partial T}{\partial \tau} + \text{div}(\mathbf{u} T) - \frac{1}{\text{Re} \cdot \text{Pr}} \nabla T = \frac{\partial}{\partial x_k} \left[ \frac{v_{sgs}}{\text{Pr}_{sgs}} \nabla T \right] - \frac{2}{\text{Re} \cdot \text{Pr}} u_k$$

where

$$\text{Re} = \frac{u_m R}{\nu}, \quad Gr = \frac{\beta_T g q_{sgs} R^4}{\lambda \nu^2}, \quad \text{Pr} = \frac{\rho c_p \nu}{\lambda}, \quad \text{Re}_m = 2 \text{Re}, \quad Gr_m = 16 \cdot Gr,$$

$$S_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right), \quad \beta_T = -\frac{1}{\rho} \left( \frac{\partial \rho}{\partial \tau} \right)_p$$

The classical Smagorinski model was used to calculate the subgrid viscosity:

$$v_{sgs} = \left( C_s \Delta_{sgs} \right)^2 G, \quad G = \left( 2S_{ik} S_{ik} \right)^{1/2}, \quad \Delta_{sgs} = \Delta V^{1/3}$$  \hspace{1cm} (9)
Smagorinski constant was taken equal to $C_s = 0.065$, and subgrid turbulent Prandtl number $Pr_{sGS} = 0.85$.

The calculations in this paper were carried out for constant flow rate $u_m = 1$. To maintain the constant value of flow rate at each time step the value of the mean pressure gradient $\beta_p$ was adjusted. For this purpose we used the algorithm proposed in [13] and modified to account for the volumetric power sources.

The computational domain was a cylinder with radius $L_x$ and length $L_z$. On the walls of the pipe the following conditions were set ($n$ is the internal normal to the channel wall)

$$ u_x = u_y = u_z = 0, \quad -\frac{1}{Re \cdot Pr} \frac{\partial T}{\partial n} = q_n = -\frac{1}{Re \cdot Pr}$$

(10)

At the boundaries $z = 0$, $L_z$ periodic boundary conditions were set:

$$ u(x, y, z = 0) = u(x, y, z = L_z), \quad T(x, y, z = 0) = T(x, y, z = L_z), \quad p(x, y, z = 0) = p(x, y, z = L_z)$$

In-house CFD code ANES [14] was used for the calculations. Algorithms of the code was modified for LES method and the numerical schemes of the second order were implemented. The details of the algorithms are given in [15].

For initial conditions the steady axisymmetric turbulent forced convection flow with $Gr = 0$ was numerical simulated using the $k$-$\varepsilon$ model of Launder-Sharma, implemented in the code. To create the initial content of the turbulence the velocity components were modified according to the relations:

$$ u_z = u_{00}(r) + C_k \left( \frac{2k_0(r)}{3} \right)^{0.5} r_g, \quad u_x = u_y = C_k \left( \frac{2k_0(r)}{3} \right)^{0.5} r_g, \quad r = \left[ (x - x_c)^2 + (y - y_c)^2 \right]^{1/2}$$

(11)

Here $u_{00}(r)$, $k_0(r)$ are the steady velocity and turbulent energy, $(x_c, y_c)$ are the coordinates of the center of the pipe in Cartesian, $r_g$ - random function with Gaussian distribution. For reliable creation of turbulent content, the value $C_k$ must be $2 \cdot 5$.

This paper presents the results of simulation of regimes corresponding to [7]: the regime with $Bo = 0$ and the regime with $Bo = 0.184$. The second one corresponds to highest levels of laminarization and deterioration of heat transfer due to buoyancy. Here $Bo$ is modified criterion of buoyancy:

$$ Bo = 8 \cdot 10^4 \frac{Gr_m}{Re^{3.425} Pr^{0.8}}$$

(12)

In both regimes the Reynolds number and the Prandtl number were taken equal to $Re = 2650$, $Pr = 0.7$ [7].

2.3. Mesh and solution algorithm

For simulation of axisymmetric problems the Cartesian coordinate system and the unstructured Cartesian grid with local refinement were used. First, the computational domain in the form of a parallelepiped with dimensions $L_x = 2$, $L_y = 2$ and $L_z$ (see below) was used as the base uniform Cartesian grids for unstructured Cartesian grid with local refinement and cut cells. The number of cells in the base mesh along $x$, $y$, $z$ were equal to $N_x = N_y = 32$, $N_z = 150$. At the second step a mesh refinement with three level in near-wall region was used. Each refinement level was construct from layer with 4-6 cells to smooth transition between cells of different size. All cells outside of the tube was removed from the computational domain. Finally the cells within the boundary in its volume were transformed into cut-cells to described curvilinear surface of the tube. Further work with the mesh continued as with a fully unstructured.

By default, original cell is split into 8 child cells. As shown by preliminary calculations, it would create the grid with a large number of cells (about 10 millions). Therefore, the algorithm of refinement was modified: refinement in $z$-direction was disabled. So, the cell was divided into 4 child cells and
the total number of cells amounted to 1.4 million. The calculations carried out in this work showed that such anisotropic refinement is effective.

![Grid cell computational domain.](image1)

**Figure 1.** Grid cell computational domain.

When modeling forced convection (Bo=0), the length $L_z$ is taken equal to 10. As preliminary experiments showed for simulation of mixed convection (Bo = 0.184) the value of the $L_z$ must be increased to 30. The same dimensions were used in the DNS [7].

![LES dimensionless scale.](image2)

**Figure 2.** LES dimensionless scale.

The number of cells in both variants were the same, and cell size in the $z$-axis in the case of mixed convection has increased three times. Figure 2 shows the distribution of scale $\Delta_{\text{les}}$, related to the Kolmogorov microscale $\eta_k = \left(\frac{\nu^3}{\varepsilon_0}\right)^{1/4}$, where $\varepsilon_0$ is rate of dissipation of turbulent energy obtained using RANS model.

The calculation process was divided into three stages. In the first stage, starting from initial distribution (11) the unsteady simulations during the time $\tau^{(1)} = 150 - 300$ with a time step of $\Delta\tau = 0.02$
- 0.04 was carried out. As a criterion of the quasi-steady solution the total mechanical energy of the flow $E_k$ was used.

$$E_k = \frac{1}{V_d} \int \frac{u_x^2 + u_y^2 + u_z^2}{2} dV$$

(13)

In the second stage ($\tau^{(2)} = 50 - 150, \Delta \tau = 0.02$) the time averaging of the fields is produced:

$$\bar{F} = \frac{\sum_{i=1}^{N} F_i}{N}, \quad \bar{F}_{12} = \bar{F}_{1} \cdot \bar{F}_{2}$$

where $N$ is the number of steps in time at the stage of averaging. The third step is the spatial averaging along $z$ coordinate and angle $\phi$ cylindrical coordinate system.

As in [7] and in this paper different definitions of dimensionless temperature are used, the our results of simulation were recalculated for comparison with DNS data [7]:

$$\bar{\theta} = \frac{t_w - \bar{t}}{t_w - t_m} = \frac{T_w - \bar{T}}{T_w}, \quad \theta_{rms} = \left( \frac{\theta' \theta'}{\bar{\theta}^2} \right)^{1/2} \Rightarrow \frac{(T' T')^{1/2}}{T_w}, \quad q_{t,k} = u_k^* \theta' \Rightarrow \frac{u_k^* T'}{T_w}.$$

$$u^*_z = \frac{\bar{u}_z}{u_\tau}, \quad y^+ = \text{Re} \cdot (1 - r), \quad \theta^+ = \frac{d_w}{u_\tau} \bar{\theta}, \quad u_\tau = \bar{t}_w^{1/2}$$

Here $\bar{t}_w$ and $\bar{T}_w$ are the shear stress and the average wall temperature averaged in time and over tube surface. As integral parameters for comparison the coefficient of friction $C_f$ and Nusselt number $Nu$ are used: $C_f = 2u_\tau^2, \quad Nu = \frac{2}{\bar{T}_w}$

3. Results

Comparison of the integral parameters of DNS [7] and LES of this work is shown in table 1. Comparisons of averaged fields are shown in figures 3 - 6. In all the figures lines correspond to the DNS, and markers to LES, $1 - \text{Bo}=0; \quad 2 - \text{Bo}=0.184$. 

![Figure 3a. The velocity profile in the global coordinates.](image1.png)

![Figure 3b. The velocity profile in wall coordinates.](image2.png)
Table 1. The integral parameters of the flow.

| Variable       | Bo = 0       | Bo = 0.184  |
|----------------|--------------|-------------|
|                | DNS          | LES         | DNS          | LES         |
| \(C_0\)        | 9.38 \times 10^{-3} | 9.73 \times 10^{-3} | -            | -           |
| \(C_f\)        | -            | -           | 7.8 \times 10^{-3} | 7.8 \times 10^{-3} |
| \(C_d/C_f\)    | 1            | 1           | 0.84         | 0.8         |
| \(Nu_0\)       | 18.3         | 19.3        | -            | -           |
| \(Nu\)         | -            | -           | 7.5          | 8.56        |
| \(Nu/ Nu_0\)   | 1            | 1           | 0.41         | 0.46        |

Figure 4a. The intensity of velocity fluctuations \(u_z\).

Figure 4b. Resolved shear stress \(\tau_{r,z} = u'_r u'_z\).

Figure 5a. The temperature profile in the global coordinate.

Figure 5b. The temperature profile in wall coordinates.
Figure 6a. The intensity of temperature fluctuations $\theta_{rms}$.

Figure 6b. Resolved radial heat flux $q_{r,r} = \theta' u'_r$.

Figure 7. Isosurface Q criterion ($Q = 0.05$), colored by $\omega_z$.

It can be seen that a good agreement between LES and DNS was obtained. An important result is that the LES model describes well the process of reduction in turbulent transport of momentum and energy due to buoyancy. Figure 7 shows the surface of constant Q criterion, colored by the value of the $z$-components of vorticity vector:

$$Q = \frac{1}{2} (\Omega'_a \cdot \Omega'_a - S'_a \cdot S'_a), \quad \Omega'_a = \frac{1}{2} \left( \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x} \right), \quad \omega_z = \frac{\partial u_x}{\partial y} - \frac{\partial u_y}{\partial x}$$
It can be seen that the number of vortices is dramatically reduced, and their shape becomes more elongated.

4. Conclusion
The comparison of LES and DNS results shows that the use of LES on unstructured grids with local anisotropic refinement allow to describe the effect of buoyancy on turbulence and heat transfer in upward heated flow.

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