Aerosol Migration by Turbulent Natural Convection in an Enclosure

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Summary
This work is performed in the frame of the study of the behaviour of aerosols in a reactor containment in case of sodium fire on the floor. Several physical effects rule the concentration of aerosols in the containment, as the source term due to the combustion, agglomeration of particles, sedimentation and wall deposition. The topic of the paper is the study of the effect of transportation of particles, due to natural convection, on the concentration and deposition kinetics.

If we assume that the concentration of aerosols has no influence on the flow pattern, the problems of flow and concentration calculations can be uncoupled.

The flow and heat transfer has been calculated in a cylindrical enclosure with given wall temperature i.e : \( T = 0 \) everywhere except on the central region of the floor where \( T = 1 \). Thermal and geometrical conditions has been varied through the Rayleigh (Ra) number for a constant Prandtl number (Pr = 0.7).

The code used solves the momentum equations for the primitive variables velocity and pressure, with a mixed finite element interpolation.

The laminar flow is calculated for Ra comprised between \( 10^6 \) and \( 4 \times 10^6 \). The local heat fluxes are calculated on the boundary and a correlation for global heat transfer is proposed.

The turbulent flow calculation is performed at \( Gr = 4 \times 10^{10} \) with the help of two turbulence models:

- The one equation K-\( \varepsilon \) model, for the turbulent energy \( K \) and fixed length scale
- The two equation K-\( \varepsilon \) model for turbulent energy and dissipation rate \( \varepsilon \).

For both calculations, use is made of the wall functions technique.
I. Introduction

This study was motivated by reactor safety considerations. The work has been performed in the frame of more general study, on the behavior of aerosols in a reactor containment, in case of sodium fire on the floor. The filter design depends upon the knowledge of the aerosol concentration in the containment as a function of space and time. The objective of the study is to determine the influence of convection on aerosol transport and deposition.

As a first step, we present in this paper the numerical simulation of the turbulent flow induced by a fire and comment the results. The steady state flow is considered in a vertical circular cylinder, with the fire simulated by a constant temperature heat source, located at the center of the floor.

The finite-element Tethys-code has been used to predict the turbulent flow using primitive variables in cylindrical coordinates with both, a one-equation turbulent model (K-ε) and a two-equations model (K-ε).

The numerical schemes used are based on the schemes developed by Taylor and Hood [1], and Bercovier [2].

The governing equations are presented in § 2. In § 3, we present a new technique for the wall function calculation in free convection, followed by a description of the numerical method used (§ 4). The results are presented and discussed in § 5.

II. Governing equations

Let us consider the steady state buoyant flow of air within a vertical cylinder (2 m. high, 2 m. diameter). These dimensions have been chosen because an experimental validation is planned in such a cylinder. The fire is simulated by a circular hot spot (radius : 0.2 m) centrally located on the floor at the temperature $T_0$. All elsewhere the walls are isothermal at the temperature $T_0$. The flow is assumed axisymmetric (cf. fig. 5). The fluid properties are kept constant except the density for the buoyancy forces (Boussinesq approximation).

Air has a very little heat capacity. The heat absorbed by the air is a small fraction ($\sim 1\%$) of the total energy produced by the fire. Therefore the temperature level within the vessel is strongly dependent upon the heat transfer to the walls. The radiation heat transfer has been neglected.

The equations are solved in a dimensionless form using cylindrical coordinates.

$$
\frac{\nu}{R} = \frac{u}{u_0}, \quad \frac{\theta}{\Delta T} = \frac{T - T_0}{\Delta T}, \quad \frac{\nu^2}{\rho_0 u_0^2} = \frac{P - \rho_0 g \Delta T Z}{\rho_0 u_0^2}
$$

$R$ = radius of the vessel
$R$ = height of the vessel
$R_S$ = radius of the source
$T_S$ = source temperature
$T_0$ = wall temperature
$\Delta T_0$ = $T_S - T_0$
$u_0 = \sqrt{g \Delta T_0 R_0}$ : unit of velocity
$Gr = \frac{g \Delta T_0 R_0^3}{\nu^2}$ : Grashof number
$Pr = \frac{\nu}{\alpha} = 0.71$ : Prandtl number

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In the laminar case the momentum, mass conservation and energy equations are:

\[
\begin{aligned}
\sqrt{\text{Gr}} \ u_j \frac{\partial u_j}{\partial x_j} + \frac{1}{\text{Pr}} \frac{\partial T}{\partial x_j} - \frac{u_j}{r} \frac{\partial}{\partial r} \delta r &= \frac{\partial}{\partial x_j} \left( \frac{\partial T}{\partial x_i} \right) \eta_i (\eta_i = \left| \frac{g_j}{g} \right|) \\
\end{aligned}
\]

(1)

This dimensionless form shows an asymptotic dependency of the velocity with \(\sqrt{\text{Gr}}\) for large Grashof numbers.

In the turbulent case the equations are:

\[
\begin{aligned}
\sqrt{\text{Gr}} \ u_j \frac{\partial u_j}{\partial x_j} &= \frac{3}{\text{Re}_p} \left[ (1 + \frac{\nu}{\nu_T}) \frac{\partial u_j}{\partial x_j} \right] - \frac{u_j}{r} \frac{\partial}{\partial r} \delta r - \sqrt{\text{Gr}} \frac{\partial T}{\partial x_i} + \sqrt{\text{Gr}} \ \eta_i \\
\end{aligned}
\]

(2)

\[
\begin{aligned}
\eta_i &= \frac{u_j}{r} \frac{\partial}{\partial r} \delta r = 0 \\
\sqrt{\text{Re}_p} \ u_j \frac{\partial \eta_j}{\partial x_j} &= \frac{3}{\text{Re}_p} \left[ (1 + \frac{\nu}{\nu_T}) \frac{\partial \eta_j}{\partial x_j} \right] \\
\sqrt{\text{Gr}} \ u_j \frac{\partial \eta_j}{\partial x_j} &= \frac{3}{\text{Re}_p} \left[ (1 + \frac{1}{\sigma_k}) \frac{\nu}{\nu_T} \frac{\partial \eta_j}{\partial x_j} \right] + \frac{\nu}{\nu_T} - \sqrt{\text{Gr}} \ \eta_j \\
\sqrt{\text{Gr}} \ u_j \frac{\partial \eta_j}{\partial x_j} &= \frac{3}{\text{Re}_p} \left[ (1 + \frac{1}{\sigma_E}) \frac{\nu}{\nu_T} \frac{\partial \eta_j}{\partial x_j} \right] + C_1 \frac{\nu}{\nu_T} \eta_j - C_2 \sqrt{\text{Gr}} \ \eta_j \\
\end{aligned}
\]

\[k = \frac{\nu}{\nu_T} \frac{U^2}{O} \]

The turbulent kinetic energy

\[E = \frac{1}{3} \frac{\nu}{\nu_T} \frac{U^3}{O} \]

The energy dissipation rate

\[\frac{\nu}{\nu_T} \left[ \frac{\partial u_j}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] + 2 \frac{\nu}{r} \frac{\partial}{\partial r} \delta r \]

\[\frac{\nu}{\nu_T} \left[ \frac{\partial u_j}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] = C_1 \frac{\nu}{\nu_T} \eta_j - C_2 \sqrt{\text{Gr}} \]

For the one-equation model \(E\) is locally determined by the relation \(E = C_D \frac{\nu}{\nu_T} \frac{U^3}{O} \)

instead of using the \(E\)-equation.

\(L\) : length scale, kept constant in the domain \(L = \frac{0.20}{O} \) and \(\frac{\nu}{\nu_T} = C' \sqrt{\text{Gr}} \ \eta_j \ \eta_j \)

For the two-equations model \(K-E\)

\[\frac{\nu}{\nu_T} = C_2 \frac{\nu}{\nu_T} \sqrt{\text{Gr}} \]

The constants of the turbulence models are:

\[\begin{array}{c}
-136- \\
B 3/2
\end{array}\]
\[ C_D = 1 \quad C'_\nu = 0.09 \quad C_\nu = 0.09 \quad C_1 = 1.4 \quad C_2 = 1.92 \]
\[ C_T = 1.0 \quad C_{K} = 1.0 \quad C_\epsilon = 1.3 \]

III. Boundary conditions

In the laminar cases the boundary conditions are simple and mentioned on figures 4 & 5.

In the turbulent case we use the wall function technique. However in case of natural convection the standard wall functions (logarithmic laws) have to be modified. Along the vertical walls the buoyancy terms strongly influence the local shear stresses which are no longer constant across the boundary layer.

\[ \tau(y) = \tau_o + \int_0^y \rho g \beta (T - T_\infty) dy \]

where \( \tau = \left( \mu + \mu_s \right) \frac{3u}{\partial y} \) is the total shear stress.

The standard wall functions remain valid at very small distances from the wall, as shown on fig. 3. Otherwise the use of logarithmic laws leads to an underestimation of the wall shear stress (\( \tau_o = \rho u_+^2 \)), the heat flux and the \( K \) and \( \epsilon \) level.

The cure was a 1-D steady state computation of the boundary layer profile, in the region near the wall coupled with the elliptic finite-element procedure for the outer regions.

Let :
\[ u_+ = \frac{u}{u_*} \quad y_+ = \frac{y}{u_* / \nu} \quad \theta_+ = \frac{\theta - \theta_o}{\theta_*} \quad \Delta T = T - T_\infty \]

with :
\[ u_* = \sqrt{\frac{\rho_o u_*}{\rho}} \quad \theta_* = \frac{\phi_o u_*}{\rho C_p u_*} \]

Then the boundary layer equations can be written in dimensionless form :

\[
\frac{2}{3} \frac{\partial}{\partial y_+} \left[ \left( 1 + \frac{v_T}{v} \right) \frac{3u}{\partial y_+} \right] + \frac{\rho g \beta}{u_*} \left( 1 - \frac{\theta_+}{\Delta T} \right) = 0
\]

\[
\frac{2}{3} \frac{\partial}{\partial y_+} \left[ \left( 1 + \frac{v_T}{v} \frac{Pr}{\sigma_T} \right) \frac{3\theta_+}{\partial y_+} \right] = 0
\]

(3)

We took for the eddy diffusivity \( v_T/v \) the law proposed by Kato \( [3] \), which can be applied to either forced or free convection.

\[ \frac{v_T}{v} = 0.41 \quad y_+ \left[ 1 - e^{-0.0017 \cdot y_+^2} \right] \]

At a given iteration the boundary conditions for the 2-D computation are \( \tau_p \) and \( \phi_p \) (the shear stress and the heat flux) at a distance \( y_p \) from the wall. As shown on figure 1 the results \( u_p \) and \( T_p \) together with \( u_o \) and \( T_o \) (the wall velocity and temperature) are used as boundary conditions for the 1-D computation. The result is again \( \tau_p \) and \( \phi_p \) and so on...

If the procedure converges \( \tau_p \), \( \phi_p \), \( u_p \) and \( T_p \) are solutions for the coupled system with \( u_o \) and \( T_o \) as wall boundary conditions.

Equations (3) are solved by a finite-element method, using linear 1-D elements, for all the mesh points of the vertical wall.

The mesh for the interval \( [y_{+o}, y_{+p}] \) is logarithmic.

At \( y_+ = 1 \quad u_{+o} = y_+ \) and \( \theta_{+o} = Pr \cdot y_+ \). The law \( u_+ = y_+ \) is experimentally verified
up to $y_+ = 5$.

This leads to the following procedure:

For given $y_p$
  > Initialization of $u_+^*$ and $\theta_+^*$
  > Discretization of the interval $[y_{+0}, y_{+p}]$
  Solve:
  \[
  \begin{align*}
  (A) & \quad u_+^* = S(\theta_+^*) \\
  (B) & \quad \theta_+^* = 0
  \end{align*}
  \]
  Compute new values of $u_+^*$, $\theta_+^*$, and $y_{+p}$
  at the convergence $u_+^*$, $\theta_+^*$, $\tau_+^*$, and $\phi_+^*$

2-D computation.

Two preliminary numerical tests are presented in fig. 2 and 3.

1) Forced convection boundary layer. 2) Free convection boundary layer along a heated vertical plate. In the first case our results are satisfactory. For the second case the results show an improvement with regard to the logarithmic law but the results deviate from those of Kato. The differences are due to the convective terms, which are neglected. This discrepancy remains acceptable if we choose $y_p^* / \delta < 0.2$ ($\delta$ : boundary layer thickness).

IV. Numerical methods for the 2-D elliptic computation

The governing equations (1 and 2) are solved by a finite-element method using linear quadrilaterals for the velocity temperature $K$ and $\varepsilon$. The pressure is constant over an element. The non-linear terms are treated by a fixed point method. The linear system is divided into a matrix for $(u, p)$ and 3 matrices for the temperature $K$ and $\varepsilon$. The matrices are successively inverted by a block frontal method. The converged solution for the $K$-$\varepsilon$ model has been easily obtained. On the other hand, with the same procedure, the solution for the $K$-$\varepsilon$ model involved relaxation parameters less than 0.3, and about 3 times more iterations.

For the $K$ and $\varepsilon$ equations the source terms are treated so that the second member be always positive.

Furthermore the mass matrices are lumped.

Example:

\[
\begin{align*}
\sqrt{Gr} \quad u_j & \quad \frac{\partial W}{\partial X_j} - \frac{2}{3} \frac{\partial N}{\partial X_j} \\
\frac{\partial K}{\partial X_j} & \quad \frac{\partial N}{\partial X_j} + \frac{\partial N}{\partial X_j}
\end{align*}
\]

V. Results

a) A preliminary comparison fig. [4] has been made with the results obtained by Torrance and Rockett [4] with a cylindrical vessel $R_0 = H = 1$, and a source radius $R_S = 0.1$.

The slight discrepancy observed at $Ra = 4 \times 10^4$ is due to the discretization scheme for the convective terms (upwind scheme in the case of Torrance and Rockett, centered scheme here).

b) Laminar cases

For the geometry described in § 2 the results at $Gr = 4 \times 10^4$, $4 \times 10^5$, $10^6$ and $4 \times 10^6$ are presented in figure (6). Numerical oscillations appear at $Gr = 4 \times 10^6$ (stability limit for this mesh and centered scheme). For all the laminar cases computed the upper flow separates from the ceiling. From $Gr = 10^6$ up we observe a plume region, a vertical wall boundary layer and an intermediate region almost thermally stratified (cf. figure 7).
c) Turbulent cases

The fluid properties are kept constant at $T = 110^\circ\text{C}$ and $P = 1$ bar i.e. $\beta = 2.6 \times 10^{-3}$ and $\nu = 2.6 \times 10^{-5}$, $T_S = 1100^\circ\text{C}$ and $T_0 = 35^\circ\text{C}$. The Grashof number is $Gr = 4 \times 10^{10}$. For the K-L model the length scale $L$ is kept constant all over the domain $L = 0.2 \text{ m}$ (dimensional characteristic of the plume). The first computation presented on figure 9 has been made with a K-L model and standard logarithmic laws. We observe a high level of the temperature within the vessel ($674^\circ\text{C}, 642^\circ\text{C}$). Furthermore as shown on figure 8 the local Nusselt number along the vertical wall seems to be underestimated. For the following computations (K-L and K-ε) we used the procedure described in § 3 for the vertical wall. The improvement on the local heat transfer coefficient is clearly shown in figure 8. We took for $T_\infty$ the averaged temperature in the intermediate region.

However it remains an important discrepancy with the experimental data. The effect of the corners influences only a few mesh points. The temperature level within the vessel falls to $250^\circ\text{C}-200^\circ\text{C}$ for the K-L model and to $216-173^\circ\text{C}$ for the K-ε model (cf. fig. 10 and 11). The two models differ mainly in the outer region of the plume. We tried to compare our results in the plume region with those obtained by Nakagome [5] for a plume in an infinite quiet atmosphere.

The axial distribution of velocity shows a virtual source located 0.5 m below the bottom of the vessel. The plume region (when the axial velocity decreases) corresponds to 2 or 3 source diameters. The experiment of Nakagome corresponds to 11 source diameters.

The fact that the flow is confined can explain the discrepancy between the axial velocity and temperature and the classical laws (figure 12)

$$\frac{u}{u_{\text{max}}} \sim (z + a)^{-1/3}$$

$$\frac{T}{T_{\text{max}}} \sim (z + a)^{-5/3}$$

The radial distribution of velocity temperature and turbulent kinetic energy are in better agreement figure 13. The K-L model show an overestimation of the turbulent kinetic energy.

d) Conclusions

A finite element code has been used to predict the flow and heat transfer in an enclosure with prescribed wall temperature. Special attention has been paid to wall functions calculation. No references, neither numerical nor experimental, have been up to now published on this subject, only local verifications were made i.e in the region of the plume and concerning the heat transfer to the vertical wall.

A discrepancy remains for this heat transfer compared to known correlations for a vertical wall in infinite medium. Part of this discrepancy comes from the fact that the calculation is made in an enclosure. However the wall function calculation can be improved by taking into account the convective term in the boundary layer.

References

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Figure 4

Figure 5

Figure 6

Figure 7

Les isovaleurs précédées d'une étoile (*) sont à multiplier par $10^9$. 

Figure 7