COMPUTATIONAL SIMULATION OF TURBULENT NATURAL CONVECTION IN A VOLUMETRICALLY HEATED SQUARE CAVITY

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Abstract *This work aims to analyze the turbulent natural convection in a volumetrically heated fluid with similar characteristics of an oxide layer of a molten core in the lower head of the pressure vessel. The simulations were carried out in a square cavity with isothermal walls, for Rayleigh numbers (Ra) ranging from* 10^9 *to* 10^{11}*. Different turbulence models based on Reynolds Averaged Navier-Stokes equations were studied, such as the standard* $k-\varepsilon$*, low-Reynolds-*$k-\varepsilon$ *and Shear Stress Transport (SST), using the open-source Computational Fluid Dynamics (CFD) code - OpenFOAM (Open Field Operation and Manipulation). The results of the three turbulence models were compared versus the results of experimental correlations and other authors' simulations, and the conclusion was that the most promising model proves to be the SST, due to its accuracy and robustness.*

Keywords: *Natural Convection, Severe Accident, Turbulence Model*

1. NOMENCLATURE

c_p	constant pressure specific heat (J/kgK)
h	convective heat transfer coefficient (W/m^2K)
k	turbulent kinetic energy (m^2/s^2)
L	length (m/s^2)
Nu	Nusselt number (hL/λ)
Pr	Prandtl number (ν/α)
q_v	volumetric heat generation (W/m^3)
Ra	Rayleigh number ($\beta g L^5 q_v/\alpha\nu\lambda$)
t	time (s)
T	temperature (K)
u_τ	friction velocity (m/s)
U_i	velocity vector (m/s)
V	component y velocity (m/s)
y^+	dimensionless wall distance ($c_\mu^{1/4}k^2/\nu$)

Greek Symbols

α	thermal diffusivity (m^2/s)
ϵ	dissipation rate of turbulent kinetic energy (m^2/s^3)
λ	thermal conductivity (W/ms)
nu_t	turbulent viscosity (m^2/s)
nu	kinetic viscosity (m^2/s)
ρ	specific mass (kg/m^3)
τ_w	wall shear stress (kg/ms^2)

Subscripts

i	finite volume boundary index
v	volumetric

2. INTRODUCTION

Severe accident (SA) in a nuclear reactor, such as the one which occurred at Three-Mile Island, Chernobyl in the eighties and very recently Fukushima, is defined as the event which features significant degradation of the reactor core. SAs are invariantly associated with loss-of-coolant, leading to overheating of the core, and eventually to meltdown of nuclear fuel (UO_2) and fuel cladding (Zircaloy). The molten mixture of fuel and cladding (corium) migrates down the reactor, reaching the lower plenum of the pressure vessel. If it is assumed the corium stays there, i.e. it does not melt the walls of the reactor vessel and migrates outside the vessel, natural convection of the corium occurs, due to the decay heat released by fission products still present in the corium.

The range of phenomena taking place in the corium at the lower plenum is immense. Working fluid is a non-homogeneous multiphase mixture of a number of elements, with intense internal heat generation, interaction with the walls of the reactor vessel, wall degradation, to name a few of the most important phenomena. The motivation for this work is the importance of the natural convection in determining of the total thermal load in the lower head vessel after a core meltdown accident and the mid-term goal of this work is modeling of natural convection in the corium, assuming the mixture is homogeneous, Newtonian, and assuming there is no phase change.

Even with such strong assumptions, modeling of the flow is not straightforward. Rayleigh numbers are rather high (up to 10^{17}) which poses challenge to existing turbulence models due to a number of factors. First of all, such flows are inherently unsteady. Second difficulty is the treatment of the near wall regions. Wall functions are hardly the answer, since the boundary layer regions are in constant transition, due to flow configuration and inherently unsteady nature of the flow. Finally, the production of turbulent kinetic energy due to buoyancy should be modeled properly. In order to select the most appropriate turbulence model for natural convection modeling in corium, the performance of k-ε, SST and Launder Sharma (LS) variant of k-ε was assessed for the known flow of internally heated fluid in a square cavity.

Results obtained by the three turbulence models were compared against the results of experimental correlations and other numerical simulations, and it can be noted that the most promising model proves to be SST, due to its accuracy and robustness. All models predict unsteady flow patterns, which are also shown and discussed in this paper.

2.1 Bibliography review

As explained above, the study of natural convection in a molten core after a severe accident poses a significant challenge. In order to understand the nuclear reactor vessel behavior and propose accident managements, it is necessary to have a general vision of the heat transfers that are present in the volumetrically heated liquid pools, among which the natural convection exerts an essential role. So, both experimental and numerical simulation works have already been done in order to analyze this heat transfer phenomenon and the factors that can influence on it.

Despite of the difficulties in executing experiments with fluids able to support high temperatures and reproduce the conditions of severe accidents, many experimental studies on natural convection have been carried out. Kulacki (1975) studied natural convection in a horizontal fluid layer boundary bounded by upper isothermal surface and bottom insulated plate. For Prandtl numbers varing from 2.75 to 6.85 and Rayleigh numbers up to 2×10^{12}, the experimental data of Kulacki (1975) were correlated by the following expression:

$$Nu_{top} = 0.403Ra^{0.226} \tag{1}$$

Mayinger (1976) obtained numerically and experimentally average Nusselt numbers on the bottom and top surfaces of a two-dimensional semicircular slice cavity, with all cavity wall being cooled. The Prandtl number of the working fluid was 7.0 and the Rayleigh numbers ranged from 10^7 to 5×10^{10}.

Despite the fact that most experiments have been performed in semicircular slices and hemispherical cavities, there are some experiments which were done in rectangular pools. Lee *et al.* (2007), for instance, studied the natural convection in a rectangular cavity with a working fluid Prandtl number ranging from 4 to 8 for water and 0.71 for air. Different boundary conditions were studied and the influence of Pr number in both upward and downward heat transfer was also found.

Some experiments have been carried out so as to provide data to validate turbulence models. One of them is called CEA BALI, which used water as a simulant fluid in order to study natural convection under internal Rayleigh number, ranging from 10^{15} to 10^{17}. This experiment was more detailed by Bonnet (1999) and it was applied in the analysis of some turbulent models carried out by Fukasawa *et al.* (2008).

Many numerical works have been developed in order to reproduce some experiments and also to provide an insight of the phenomena associated with the molten core. However it is certain that the numerical simulations are also challenging. To enable the effects of turbulence can be predicted, a great amount of CFD research has been focused on methods which make use of turbulence models.

Dol and Hanjalic (2001) performed $2D$ and full $3D$ computations with low-Reynolds-number $k - \varepsilon$ models (KEMs) to simulate the natural convection in a side-heated near-cubic enclosure containing dry air ($Pr = 0.71$) under Rayleigh number equal to $Ra = 4.9 \times 10^{10}$.

The validation of k-ϵ, k-ω, SST and a coarse DNS models for turbulent natural convection in a differentially heated cavity containing a fluid with $Pr = 0.71$ and Rayleigh numbers ranging from 1.58×10^9 to 10^{12} was performed by Aounallah *et al.* (2007). The conclusion of Aounallah *et al.* (2007) was that the k-ω-SST provided superior outcomes than the other models analyzed, though it was not able to reproduce accurately the mean flow.

Due to the presence of different materials inside the vessel head, it is difficult to know exactly the value of the Prandtl number of the molten core. Thereby, some studies have been realized in order to understand the influence of fluid properties on the heat transfer behavior. In this context, Nourgaliev *et al.* (1997) investigated the effect of Prandtl numbers, varying from 0.2 to 7.0, in cavities with different geometries (rectangular, semicircular, hemispherical and elliptical). It was observed an increase of Nu number as the Ra number raised and the most influence of Pr number in the bottom of the cavities.

Both the analysis of the influence of Pr number and the adequate application of CFD methods for the development of security analysis tools were part of the work performed by Tran *et al.* (2010). The turbulence model used was the $ILES$, which provided outcomes in agreement with Kulacki and Emara (1977) empirical correlations and it was able to scrutinize the enforceability of the simplified model ECM.

This brief bibliography review aimed to approach some experimental works that have been done since the seventies, for example, until recently and are still used as a way of comparison for numerical simulations. With the help of CFD tools it could be noted that several numerical simulations have placed an important role for the natural convection study, contributing also to the management of nuclear safety.

3. Mathematical Model

In this section, the physical problem will be presented, as well as the governing equations and the numerical procedure adopted to solve them.

3.1 Geometrical considerations

A volumetric heated square cavity with all isothermal walls (at $T = 273K$), representing the external cooling of the vessel, containing a working fluid Pr number equal to 0.6 is the physical problem used for the natural convection study with Ra numbers ranging from 10^6 to 10^{11}.

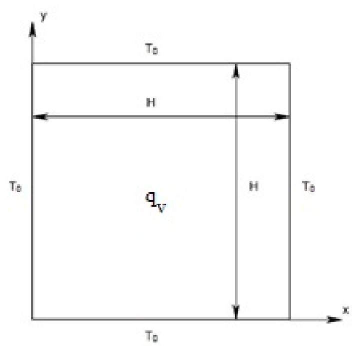


Figure 1. Scheme of the physical problem

For all the calculations presented in this work, a uniform grid 100×100 was used, which was previously chosen in a mesh sensitivity analysis.

3.2 Governing equations

The Reynolds-Averaged Navier-Stokes (RANS) for mass, momentum and energy conservation equations for buoyancy driven incompressible flow with internal heat generation (assuming the Boussinesq approximation), can be written respectively as:

$$\frac{\partial U_i}{\partial x_i} = 0, \tag{2}$$

$$\frac{\partial \overline{U_i}}{\partial t} + \overline{U_j}\frac{\partial U_i}{\partial x_j} = -\frac{\partial P}{\partial x_i} + \nu\frac{\partial^2 U_i}{\partial x_j^2} - \frac{\partial \overline{u_i' u_j'}}{\partial x_j} - \beta(\overline{T} - T_0)g_i \tag{3}$$

$$\frac{\partial \overline{T}}{\partial t} + \overline{U_j}\frac{\partial T}{\partial x_j} = \alpha\frac{\partial^2 T}{\partial x_j^2} - \overline{u_j' T'} + \frac{q_v}{\rho c_p} \tag{4}$$

The turbulent stress $\overline{u_i' u_j'}$ is given by the Boussinesq hypothesis as follows:

$$\overline{u_i' u_j'} = \nu_t \frac{\partial U_i}{\partial x_j} \tag{5}$$

and the turbulent heat flux is given by:

$$\overline{u_i' T'} = \alpha_t \frac{\partial T}{\partial x_i} \tag{6}$$

Both the turbulent stress and turbulent heat flux represent the unresolved turbulence contributions, which need to be modeled in order to close the above equations. So, this paper adopted three different RANS turbulence models to close the system of equations: the $k - \varepsilon$, SST and low-Reynolds number model - Launder-Sharma (LS). All of these models are based on the Reynolds analogy, which relates the eddy viscosity and the turbulent thermal diffusivity by the turbulent Prandtl number (Pr_t), according to the following equation:

$$\nu_t = Pr_t \alpha_t \tag{7}$$

in which, nu_t is determined by the turbulent kinetic energy (k) and its dissipation rate (ε):

$$\nu_t = C_\mu \frac{k^2}{\varepsilon} \tag{8}$$

The discretized set of equations is solved by the finite-volume solver OpenFOAM, for two-dimensional buoyant flow. The PIMPLE algorithm is applied for coupling between the velocity and pressure fields. For spatial discretization of all terms, the second order accurate central difference scheme was used, whereas time integration was performed with the implicit backward Euler method.

4. RESULTS AND DISCUSSION

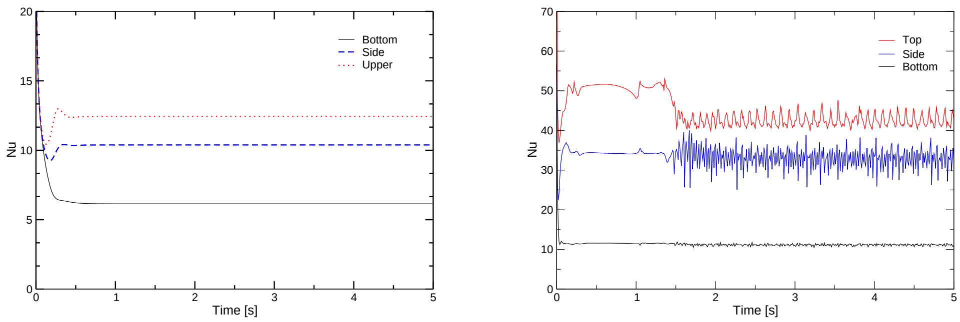
The fluid used in the simulations has Prandtl number equal to $Pr = 0.6$, at the same order of magnitude for an oxide material(Theofanous *et al.* (1997)). It is certain that there is a considerable number of experiments concerned with natural convection in spherical cavities. However, according to Horvat *et al.* (2001), studies comparing the experimental outcomes of natural convection in rectangular and spherical cavities show some similarity between them. So, in order to scrutinize the natural convection phenomenon, a simple geometry (square cavity) was chosen, with boundary conditions representing the cooling of the molten core, this is all walls with a constant temperature at 0^o C (273 K).

The mesh was generated with ICEM CFD software and then exported to OpenFOAM. Three RANS models was used in the simulations, k-ε, SST and LS. The computational simulations were carried out for Rayleigh numbers ranging from 10^6 to 10^{11}. As it can be observed in Figure 2-(a), at $Ra = 10^6$ the simulation is laminar and reaches a steady state, contrary to the case at $Ra = 10^9$,Figure 2-(b), for which the regime is transition to turbulence. On the top wall the heat transfer is more intensive because the fluid flow towards to the upper surface which is at a low temperature. Then the fluid flows to through the side walls transferring heat until reaching the bottom wall with a considerable low temperature and consequently the heat transfer on the bottom is less than through other walls.

At $Ra = 10^6$ the flow is symmetric, but as the Rayleigh number increases the symmetry is lost and the regime starts to be transient and unstable. First instabilities can be observed at $Ra = 10^8$.

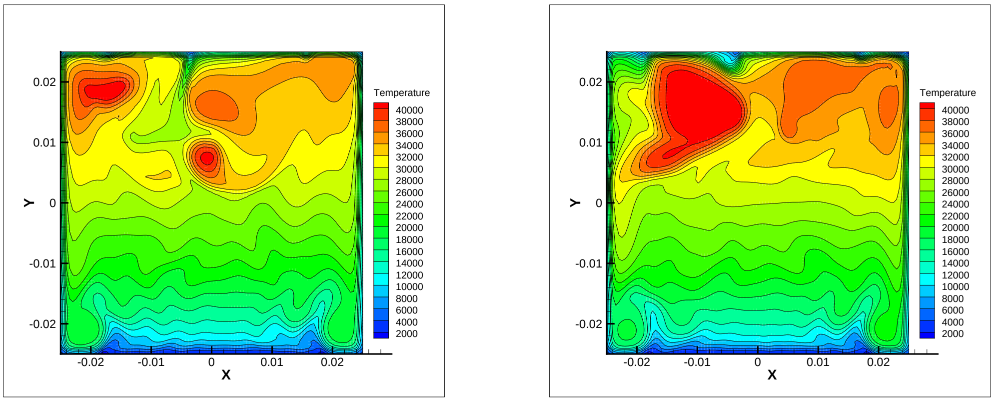
According to Figure 2, it can be observed that LS model overpredicted Nusselt number on the top, region in which the flow reaches after the fluid has been heated. The reason for that phenomenon is due to the fact that both low and high $k - \varepsilon$ are not adequate to predict accurately the level of turbulent kinetic energy in the stagnation region and consequently the Nusselt number is also dramatically overpredicted on that same region (Craft *et al.*, 1993).

By means of the temperature and vertical velocity fields depicted by Figures 3 and 4, it can be noted that the highest temperature occurred on the top wall and a squeezed fluid flow appeared next to the side walls and, for the highest Rayleigh number ($Ra = 10^{11}$), the simulation was highly unstable, presenting many unsteady structures in the fluid flow and related heat transfer.



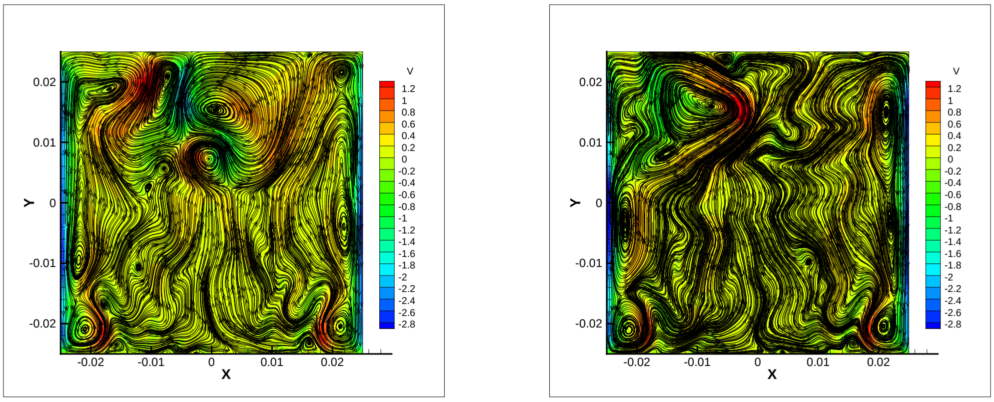
(a) (b)

Figure 2. Boundary averaged Nusselt provided by LS model for $Pr = 0.6$ at (a) $Ra = 10^6$ and (b) $Ra = 10^9$



(a) (b)

Figure 3. Temperature field computed with SST for $Pr = 0.6$ and $Ra = 10^{11}$ at (a) 1500s and (b) 6000s

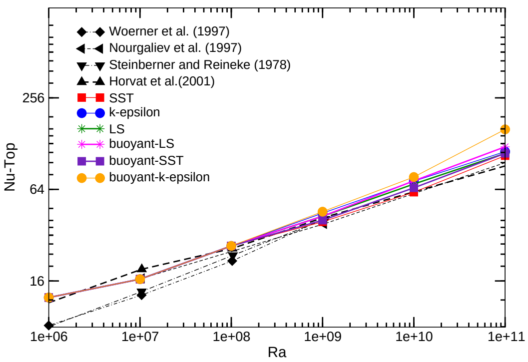


(a) (b)

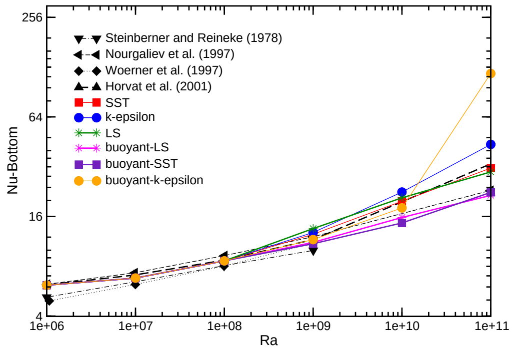
Figure 4. Vertical velocity field computed with SST for $Pr = 0.6$ and $Ra = 10^{11}$ at (a) 1500s and (b) 6000s

According to the Figure 5, the SST results are in a good agreement with the experimental and numerical outcomes provided by other authors. The simulation with k-ε proved to be unstable during the simulation, leading to frequent crashes and necessities to perform restart. Simulations with LS model showed similar behavior, yet the crashes were less frequent than with k-ε. An interesting fact was observed with LS model, which was not predicting the turbulence before the insertion of the buoyancy production term (Gb) into the turbulent kinetic energy and dissipation rate of kinetic energy transport equations. The presence of Gb in SST and $k - \varepsilon$ equations was also analyzed (which was called as buoyant-SST and buoyant-$k - \varepsilon$, as weel as LS was defined as buoyant-LS after the Gb presence in the model), but for SST no such difference was noted and for $k - \varepsilon$ the results became even worst at Rayleigh number simulations, according to Figure 5.

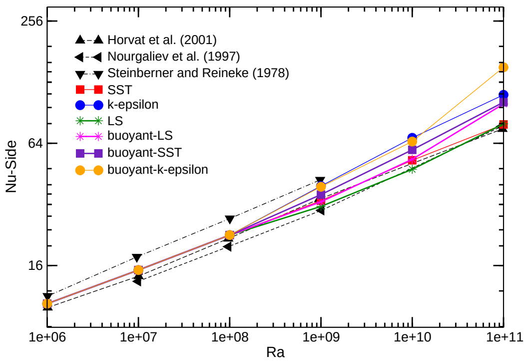
The boundary averaged y^+ values show that SST and LS are in agreement with Casey and Wintergerste (2000), since the values are not superior to 5, fact that can be observed by Table 1, which shows the $y+$ values provided by each turbulence model studied, for $Ra = 10^{11}$. The y^+ provided by k-ε simulations are also adequate for this kind of turbulence model, which does not integrate the equations up to the wall, since it makes use of wall function and consequently does not require a fine grid clustering in the near-wall region.



(a)



(b)



(c)

Figure 5. Average Nusselt numbers as a function of Ra numbers for $Pr = 0.6$ at :(a) the top wall, (b) the bottom wall and (c) the side wall.

Table 1. Boundary averaged y^+ provided by SST, k-ε and LS, for $Ra = 10^{11}$

Boundary	SST	k-ε	LS
TOP	0.34531	41.484	1.9985
LEFT	1.27844	43.14	0.92655
RIGHT	1.32941	40.9918	2.63924
BOTTOM	0.141714	42.7301	0.19479

5. CONCLUSIONS

In this work, the natural convection in a square cavity with all isothermal walls, containing a fluid $Pr = 0.6$ for Ra numbers ranging from 10^6 to 10^{11} was analyzed. Three turbulence models based on RANS equations were investigated: k-ε, SST and LS, a low-Reynolds-k-ε model. The simulations showed that the best turbulence model was SST, by the fact to be more robust, while k-ε proved to be totally unstable during the simulation, leading to frequent crashes and necessities to perform restart, specially for the simulations at high Rayleigh number. Simulations with LS model showed similar behavior, yet the crashes were less frequent than with k-ε.

The time distributions of the boundary-averaged Nusselt numbers showed that the turbulence appeared first at the side and upper walls, whereas the fluid in the lower region present more resistance for the initial of turbulence.

The buoyancy production term proved to be essential for LS model to become more robust and also to predict the turbulence, fact noticed by the very low values of $y+$ provided before its presence in the model, which is calculated based on the turbulent kinetic energy. For SST, the buoyancy production did not make any considerable difference in the results and for $k - \varepsilon$, the simulations only became more robust for low Rayleigh number.

6. ACKNOWLEDGEMENTS

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