Numerical Investigation of Turbulent Natural Convection Heat Transfer in an Internally-Heated Melt Pool and Metallic Layer

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Abstract. This paper presents results of numerical investigation of turbulent natural convection in an internally-heated oxidic pool; and in a metallic layer heated from below and cooled from top and sidewalls. Emphasis is placed upon applicability of the existing heat transfer correlations (obtained from simulant-material experiments) in assessments of a prototypic severe reactor accident.

The objectives of this study are (i) to improve the current understanding of the physics of unstably stratified flows, and (ii) to reduce uncertainties associated with modeling and assessment of natural convection heat transfer in the above configuration.

Prediction capabilities of different turbulence modeling approaches are first examined and discussed, based on extensive results of numerical investigations performed by present authors. Findings from numerical modeling of turbulent natural convection flow and heat transfer in melt pools and metallic layers are then described.

1 Introduction

In a hypothetical severe accident scenario in a LWR, core melt may relocate to, and accumulate in the reactor pressure vessel (RPV) lower plenum. Decay heating in the core melt may cause formation of a melt pool. In addition, latter relocations of metallic structure and/or separation of metallic, lighter, component from the oxidic debris may lead to formation of a metallic layer on top of the oxidic pool.

Natural convection in the decay-heated core melt pool and in the metallic layer have a profound impact on the thermal loadings of the lower head and the upper structures in the vessel. For reactor situations, the natural convection flow regimes are characterized by the very high Rayleigh numbers, due to both the large geometry scale, H, and the high heat generation rate q_v, ($Ra \sim H^3$ or $Ra' \sim H^5$). For prototypic conditions, the $Ra' = 10^{15}$-10^{17} and the flow regime is highly turbulent.

A number of experiments and analyses have been performed to study turbulent natural convection phenomena. On the experimental front, except for the RASPLAV test, the experiments have utilized simulant materials. It is difficult to realize experiments with the prototypic high Rayleigh numbers and prototypic boundary conditions. Similarly, it is difficult to model analytically turbulent pool behaviour at high Rayleigh numbers. Existing single-point closure turbulence models were found to be incapable of predicting flow and heat transfer in a situation which involves both stable stratification and unstable stratification regions (Dinh and Nourgaliev, 1997 [1], Nourgaliev and Dinh, 1996 [2]).

Numerical analyses of flows and heat transfer in this area remain, however, important, since they may help to achieve a better understanding of the role of different factors and to assure applicability and relevance of experimental data and correlations to prototypic reactor accident conditions. The objectives of numerical

modeling of turbulent flows and heat transfer in a core melt pool and a metallic layer are:
- to gain insight into physics of governing mechanisms;
- to examine effect of non-prototypical conditions in simulant-material experiments; and
- to develop a reliable prediction method, which can first be used to sastifactorily analyze the experiments performed so far, then, be applied to reactor-scale predictions.

The present study reports new results and reviews the progress in the field of turbulence modeling accomplished after the previous OECD/CSNI specialist meeting (Grenoble, 1993) on this topic.

2 Assessment of various turbulence models

2.1 $k-\epsilon$ turbulence models

A wide variety of models have been utilized to describe turbulent fluctuations in natural convection heat transfer. The available models can be divided into the following categories:
1. Algebraic model of turbulence
2. One-half equation model of turbulence
3. One-equation model of turbulence
4. Two-equation turbulence models
(a). Standard $k-\epsilon$ model using wall functions (KEM)
(b). Low-Reynolds-number $k-\epsilon$ model (LRN KEM)
(c). Modification of LRN KEM for buoyancy-driven flows
5. Reynolds stress models (RSM)
(a). Algebraic stress model (ASM)
(b). Partial differential stress model (DSM)
6. Multiple-time-scale models
7. Large-eddy simulation (LES)

Besides the above models, direct numerical simulation (DNS) has also been employed to describe transient flow field during turbulent natural convection.

In a previous study, capabilities of different modeling methods were reviewed and discussed with respect to turbulent natural convection in a large volumetrically-heated liquid pool (Dinh and Nourgaliev, 1997 [1]). The KEM, perhaps the most widely used turbulence model, employs the eddy-diffusivity concept to model the Reynolds stresses and turbulent heat fluxes. This concept describes turbulence as a diffusion process characterized by a locally isotropic turbulent viscosity. A strict analogy between the Reynolds stresses and turbulent heat fluxes is assumed, since the turbulent Prandtl number Pr_t is assumed as constant in the $k-\epsilon$ approach. It was found that at least a low-Reynolds-number $k-\epsilon$ model (LRN KEM) is required for modeling of flows in volumetrically-heated liquid pools. Moreover, modifications were necessary to account for the buoyancy-induced anisotropy of turbulence in such a liquid pool. Modifications based on the local Richardson number were employed (Dinh and Nourgaliev, 1997 [1]) for the turbulent Prandtl number and the near-wall viscosity, to account for the effects of density/temperature stratification on turbulence.

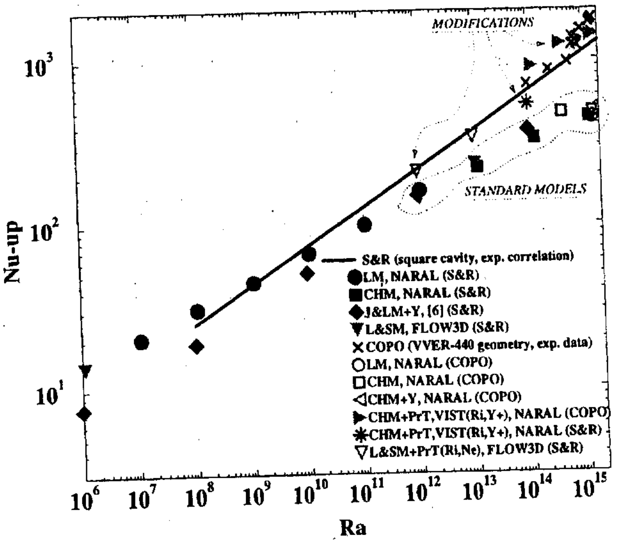

Figure 1: Variation of the average upwards Nu numbers with Ra numbers. Calculational results vs. experimental correlation of Steinberner and Reineke.

The above modifications employed in the $k-\epsilon$ model provided very good agreement with the experimental data received from the Finnish COPO-I experiments [3] and the Steinberner-Reineke [4] tests (see Fig.1). Most importantly, local heat fluxes on vertical and curved pool boundaries were correctly predicted by the model. Nevertheless, these modifications of the low-Reynolds-number $k-\epsilon$ model are experiment-specific: they cannot substitute for the fundamental deficiencies of the two-equation turbulence model.

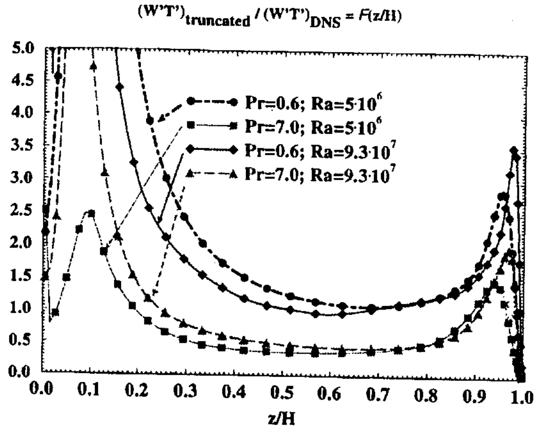

Figure 2: On applicability of the truncated algebraic form of the vertical turbulent heat flux (in case of validity, the ratio should be 1).

2.2 Reynolds-stress turbulence models

In order to account for the anisotropy of turbulence several approaches within the frame of Reynolds-stress modeling (RSM) have been developed for turbulent flow under gravitational influence. A comprehensive review of the RSM methods was provided by Dinh and Nourgaliev (1997) in ref.[1].

The decay phenomenon of a buoyant jet has been predicted from a differential $k-\epsilon-\bar{\theta}^2$ turbulence model of Chen and Rodi (see Chen and Chen, 1979 [5]). In this approach, the turbulent stresses and heat fluxes are modeled by algebraic expressions while the differential equations are solved for the kinetic energy of turbulence (k), the dissipation rate of turbulence kinetic energy (ϵ), and the fluctuating temperature ($\bar{\theta}^2$). Furthermore, algebraic flux models also have been developed for turbulent buoyant jets (Hossain and Rodi, 1982 [6]) as well as natural convection in rectangular enclosures (Hanjalić and Vasić, 1993 [7]). The major conclusion in ref. [7] concerns the modeling of the turbulent heat flux vector, which was found to strongly influence the applicability of the model to a broader class of buoyant flows. Variants of the gradient diffusion model with isotropic and non-isotropic eddy diffusivity, and corresponding components of temperature gradients, were found to produce inconsistent results.

The turbulent natural-convection boundary layer for air flowing along a heated vertical plate, as measured by Tsuji and Nagano, 1988a [8], was investigated numerically with an algebraic (ASM) and fully differential Reynolds-stress model (DSM) by Peeters and Henkes (1992) in ref. [9]. It was shown that the turbulent Prandtl number (Pr_t) is certainly not constant over the whole flow field as was also seen in experiments by Tsuji and Nagano, 1988b [10]. Problems of wall modifications and constants, with respect to sensitivity of the ASM and DSM applied to natural convection flows, were analyzed and discussed broadly in the literature. On the one hand, the universality of a model increases with its complexity, but, on the other, the more complex are the models, the greater is the amount of empirical input needed in form of empirical constants, not to mention the increase in computing time. It is known that the ASM and DSM (especially the latter) are computationally expensive, and they are also numerically very unstable which can lead to serious convergence problems. Moreover, the wall damping functions for both of these types of Reynolds-stress models have to be validated even for simple flows and their turbulence empirical constants are not yet well-established.

Nourgaliev and Dinh (1996) [2] examined the validity of various assumptions proposed and utilized in different Reynolds-stress models for description of turbulent flow and heat transfer in liquid pools with internal energy sources. Physics of fluid in unstably-stratified flow region was studied by means of direct numerical simulation (DNS) of naturally-convecting flow in internally-heated fluid layers, with a constant temperature boundary condition on the upper surface and an adiabatic boundary condition on the bottom surface. This approach enabled the determination of the top wall heat fluxes, the mean temperature fields, the distributions of Reynolds stresses and turbulent heat fluxes. The calculated turbulence parameters are analyzed with respect to Reynolds-stress type correlations. The calculated turbulent characteristics (Reynolds stresses and turbulent heat fluxes) indicate significant anisotropy of turbulent transport properties. So, the isotropic eddy diffusion approach cannot be used to describe turbulent natural convection heat transfer under unstable-stratification conditions.

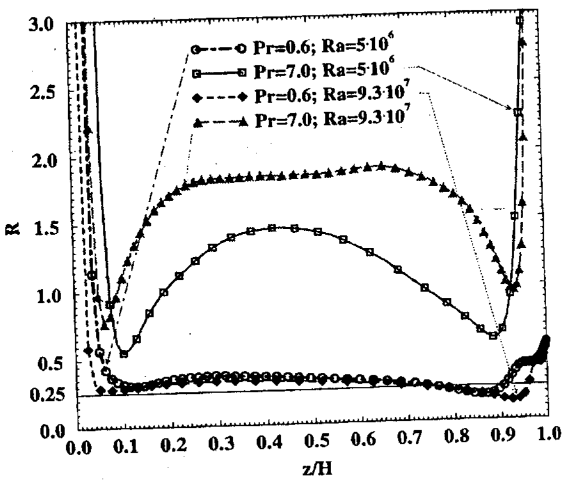

Figure 3: Dissipation time scale ratio R (proposed in RSM as constant, typically, in the range from 0.4 to 0.8).

Analysis of the thermal-variance-balance showed an important role of diffusive transport of $\overline{T'^2}$, and remarkable non-equilibrium of thermal-variance E_T. Turbulence constants, needed for modeling of turbulent diffusion, and of dissipation of thermal-variance, are strong functions of Rayleigh and Prandtl numbers, and are non-uniformly distributed in the fluid layer; see e.g. Fig.2. Fluids with two different Prandtl numbers ($Pr = 7$ and $Pr = 0.6$) were investigated. Similar turbulence statistics of the thermal fields were obtained for different Pr numbers, however, remarkably different results of turbulence statistics of the hydrofield were calculated; see Fig.3. As a consequence, important turbulence parameters and constants are found to be strongly dependent upon the fluid Prandtl number.

From the results of DNS of flows in internally-heated fluid layers, it was found that major correlations and assumptions proposed and employed in the previous Reynolds-stress modeling are violated. Thus, developing a higher order turbulence model for this type of flow, is not straightforward.

2.3 Large-eddy and direct numerical simulations

In order to produce a turbulence data base, direct numerical simulation (DNS) can be employed. In this method, the full three-dimensional time-dependent conservation equations of mass, momentum, and energy are solved on grids which resolve the largest and the smallest scales of turbulence. The calculated time-dependent flow and temperature fields can, then, be analyzed for the fluctuations induced by turbulence. In general, such a calculation has to be performed with a very fine grid structure to adequately represent the small scale turbulence in the flow fields of interest. In the past, DNS has been used for analyzing natural convection heat transfer in fluid layers with internal heat generation with low values of Ra numbers ($3\cdot10^4 \div 4\cdot10^6$) [11]. Nourgaliev and Dinh (1996) [2] performed direct numerical simulations in internally-heated fluid layers, using a finit-difference numerical scheme. A commercially available, general-purpose computer code CFX (FLOW3D) [12] was employed for calculations. Analyses were performed to evaluate grid resolution and time step requirements for the DNS calculations.

It was shown that three-dimensional formulation and proper description of mixing are mandatory in order to predict heat transfer in unstably-stratified flows. That is to say, natural convection heat transfer in these conditions is mainly governed by large eddies. Good agreement with heat transfer data was achieved

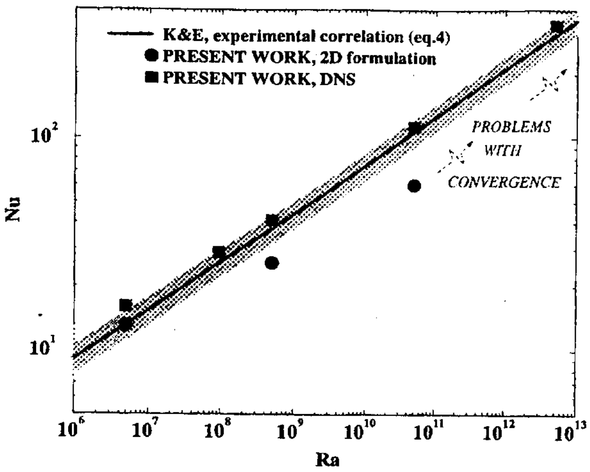

Figure 4: Prediction of Nusselt number in internally-heated fluid layers.

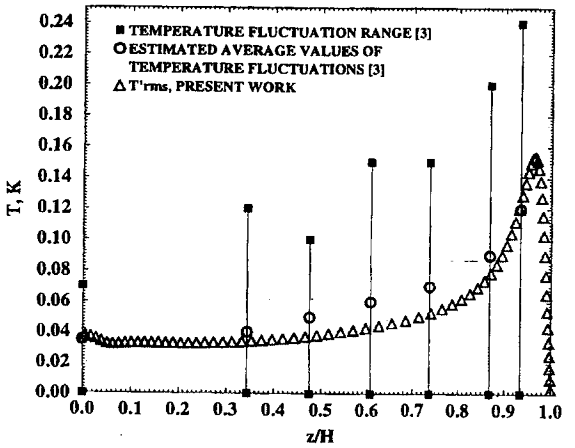

Figure 5: Temperature fluctuations: calculational results versus measurements.

for Ra numbers up to $5 \cdot 10^{12}$, but reliable turbulence data were obtained only for several Rayleigh numbers in the range $5{\cdot}10^6 \div 5{\cdot}10^8$; Fig.4. In particular, the calculated Nusselt number, temperature distributions within the fluid layer and temperature fluctuations are in good agreement with the experimental data of Kulacki et al. [13], [14]; Fig.5. Also, the calculated turbulent heat fluxes agree well with those predicted by the analytical model of Cheung [16].

Although being straightforward, DNS method has serious limitations. To resolve all scales of motion, it requires a number of grid points of N, $N \simeq L/\eta$, where L is the dimension of the computational domain and η is the smallest length scale of fluid motion. Since this ratio is proportional to $Ra^{1/3}$, the total number of grid points required by a DNS calculation in three dimensions are $\sim Ra$. For this reason, it is extremely expensive and unaffordable to perform DNS of natural convection flows in the prototypic reactor range of Rayleigh number.

To overcome the problem of limitation in computational capacity, large eddy simulation (LES) has been employed to analyze heat and mass transfer in turbulent natural convection. In LES, large scale motion is simulated whereas motion with length scale smaller than the computational grid size is modeled by a subgrid scale model (SGM). Most subgrid scale models are based on the eddy diffusivity concept, introducing an effective eddy diffusivity and conductivity for the subgrid scales.

The original subgrid scale model of Smagorinsky (1963) [17] and Lilly (1967) [18] was based on dimensional arguments and integral relations coming directly from Kolmogorov's ideas on the turbulence energy spectrum. This model assumes the isotropy of the subgrid-scale turbulence. Such an assumption may not be valid for the near-walls regions.

The subgrid-scale eddy viscosity is defined as

$$\nu_t = (C_s \cdot h)^2 \cdot S \qquad (1)$$

where h is the grid size (mesh scale), S is the scalar strain, and C_s is the Smagorinsky constant. In the literature, the constant C_s was found to vary in the range from 0.06 to 0.25 . By assuming the existence of an inertial range spectrum, Lilly (1967) [18] evaluated $C_s \simeq 0.18$.

The turbulent heat flux is often calculated by applying subgrid Prandtl number concept, Pr_{SGS}.

$$\alpha_t = \nu_t / Pr_{SGS} \qquad (2)$$

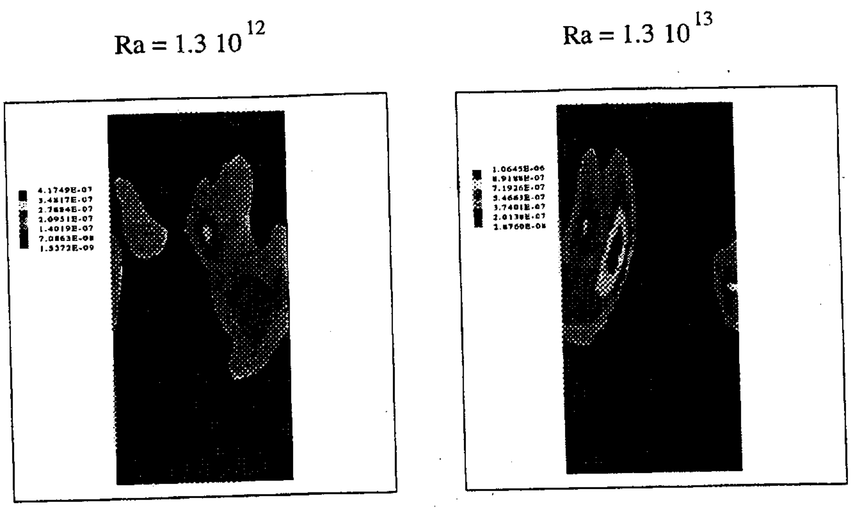

Figure 6: Typical distribution of calculated subgrid-scale kinematic viscosity in an internally heated fluid layer ($\nu = 0.8610^{-6}\mathrm{m}^2/\mathrm{s}$).

The subgrid-scale Prandtl number may depend on the fluid properties. Results of LES simulation are however less sensitive to Pr_{SGS} in fluids with the molecular Prandtl number close to one. Essentially, the model has two model constants C_s and Pr_{SGS}.

Recently, a dynamic subgrid model was proposed and developed, in which the constant C_s is not arbitrarily chosen or optimized, but computed. However, this model features numerical instability and convergence problems, and a robust numerical scheme has yet to be developed and validated.

The present authors employ the Smagorinsky-type model for LES in a large volumetrically-heated liquid pool and metallic layer. In such a pool, the core region is the major computational domain which requires huge number of computational nodes. For this region, a large eddy simulation is the most effective method. More importantly, it is found that heat transfer in large volumetrically-heated liquid pools is governed by large eddies, so that contributions from the sub-grid eddies in the mixing and heat transfer processes would remain minor, if the grid size is fine enough.

However, there appears a need in developing modification, both, for the constant, C_s, and for the subgrid Prandtl number, Pr_{SGS} in the near-wall region. In order to avoid uncertainties associated with the near-wall treatment it is proposed that the near-wall computational mesh is fine enough to resolve the smallest scales of motion, i.e. to have a combined DNS in the near-wall region with LES in the pool's core region.

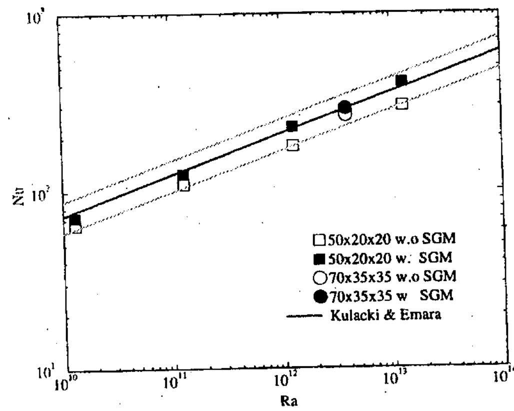

Figure 7: Comparision between simulations with and without subgrid scale model ($C_s = 0.06, Pr_{SGS} = 1$)

Both DNS and LES approaches have been developed and employed at Royal Institute of Technology (Stockholm) to analyze effects of geometry configuration, heating method, and simulant properties on turbulent heat and mass transfer in a liquid pool and a fluid layer.

3 Concluding remarks

Results of recent experimental studies of natural convection heat transfer in an internally-heated liquid pool, and in a liquid layer heated from below provide a large data base for analyses. However, there still exist significant uncertainties when extrapolating (differing) heat transfer correlations (obtained in simulant material experiments, using different geometries, using different heating methods) to prototypic reactor accident conditions. Theoretical analyses and numerical modeling are therefore necessary to evaluate sufficiency and consistency of the current data base.

Additionally, there exist other physical and chemical phenomena in a core melt pool which may affect turbulent flow fields and heat transfer. Notably, these are (i) behavior of crust at the pool's boundaries, (ii) phase change and stratification behavior of high temperature multi-component (at least, binary-oxidic) corium melts, and (iii) variation of melt physical properties with temperature and composition. These phenomena and effects should be investigated in conjunction with a reliable and generic turbulence model.

Although significant progress was made in the field of CFD applications and turbulence modeling in the past 4 years, capability and reliability of the current modeling approaches remain limited, particularly with respect to Rayleigh number conditions.

Nonetheless, it has been found that remarkable insights can be obtained from results of numerical investigations at lower Rayleigh numbers, for which the method of direct numerical simulation (DNS) is reliable and computationally affordable. Systematic examination of a particular effect for a wide Rayleigh number range (from 10^5 to 10^{12}) could provide a reliable extrapolation of the effect in reactor-scale Rayleigh numbers. This approach was extensively employed at Royal Institute of Technology (Stockholm) to perform many sensitivity and separate-effect studies.

For the purpose of reactor-scale calculations, a promising method is being developed at RIT. This method combines DNS at the wall region and large eddy simulation (LES) in the inside regions of the pool. Thus, the method has significant advantages over both the single-point closure models and the full-domain DNS approach.

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