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HIGH-FIDELITY SIMULATION-DRIVEN MODEL DEVELOPMENT FOR COARSE-GRAINED COMPUTATIONAL FLUID DYNAMICS

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ABSTRACT

Nuclear reactor safety analysis requires analysis of a broad range of accident scenarios and determining their consequences. For a nuclear power plant behavior, it is impossible to obtain experimental data at sufficiently large scales to support calibration and validation of various system models. In single-phase flow convective problems, high-resolution methods of Computational Fluid Dynamics (CFD) such as Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) can provide high fidelity results under conditions where physical measurements are unavailable. However, such high-resolution simulations are computationally expensive and not suitable for simulation of long transient scenarios in nuclear reactor accidents.

In this work, we investigate the use of a high fidelity simulation-driven approach to model sub-grid scale (SGS) effect in Coarse Grained Computational Fluid Dynamics CG-CFD. Notably, fine-mesh simulations are used to construct physics-informed statistical surrogate of coarse-mesh SGS model. For an initial analysis, we consider a case of turbulent natural convection in a volumetrically heated fluid layer with a thermally insulated lower boundary and isothermal upper boundary. This scenario of unstable stratification is relevant to turbulent natural convection in a severe nuclear reactor accident, as well as in containment mixing and passive cooling. For this type of flow, the SGS effect is modeled by an added turbulent diffusivity in the energy equation. It is shown that a global correction for the energy equation is sufficient to achieve a significant improvement to the CG-CFD prediction of thermal mixing in the fluid layer.

KEYWORDS
Turbulent Natural Convection, Coarse-grained CFD

1. INTRODUCTION

Nuclear reactor safety analysis requires identifying credible accident scenarios and determining their consequences. To achieve this goal, various model-based prediction methods are used. Increasingly, there is a need for sufficiently accurate and computationally affordable methods of Computational Fluid Dynamics (CFD) to simulate complex three-dimensional thermal-hydraulic phenomena. Despite extraordinary advances in high performance scientific computing over the past decades, traditional fine mesh CFD approaches are still computationally challenging for typically long transients in nuclear accident applications. For example, based on previous work [1], simulating steam blowdown as a part of direct containment heating scenario needed 1 week computing time on a 128-processors cluster although the mesh is not necessarily fine enough. For performing affordable simulation and capturing multi- dimensional behavior at the same time, a coarse grained CFD approach is essential. Currently many researchers are

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using various methods to do such a coarse scale simulation [2, 3], and our work is a step in the same direction.

Traditionally, CFD simulations including DNS, LES and Reynolds-Averaged Navier–Stokes equations (RANS) are computationally demanding since a wide range of length and time scales need to be resolved. Coarse-grained (CG) CFD aims to solve mass, momentum and energy equations on coarsened mesh e.g., using larger size control volumes (this way CG-CFD relates to RANS CFD in a similar relation existing between LES and DNS). This typically results in under-resolved flow, particularly vortices or boundary layers in many problems of interest. The original equations are non-linear so the challenge in CG-CFD approach is to recover the information loss in solution of the coarse grained equations so the more affordable approach still resolves the physical phenomena of interest.

One of the novel methods [2] to achieve this goal is Autonomic sub-grid closure in Large Eddy Simulation (ALES) which provides the turbulence closure without a predefined turbulence model. The ALES method expresses the local sub-grid scale stress tensor as a general unknown non-linear function of the resolved variables at all locations and all times with a Volterra series (model for non-linear behavior similar to Taylor series: here the series coefficients are computed by minimizing the error in sub-grid scale stresses at a test filter scale). Then, coefficients are mapped to LES scale assuming scale similarity (noting that both LES scale and test scale lie in the self-similar inertial range in turbulence energy spectrum). ALES method is a general model-free self-optimizing approach for turbulence simulations closure. Preliminary results [2] showed high accuracy in computing turbulent stresses compared to current turbulence models. This approach can be also used for developing new turbulence models. However, the scale similarity assumption, upon which ALES is based, is valid only in inertial range. Therefore, applying ALES in nuclear reactor safety research is still highly expensive due to large domain size compared with the turbulence scales [2].

Another approach to determine the closure model is the multilayer Neural Network (NN), which is a powerful non-linear regression technique. For example, in [3], direct numerical simulation of bubbly flow was used to find the closure term for a model of the average flow with NN. In that case, initial vertical velocity and the average bubble density are uniform except in one of the horizontal directions. As the transient develops, the bubble density and velocity become uniform. It was assumed [3] that the unknown closure term depends on the void fraction, void fraction gradient, and liquid velocity gradient. The NN approach is providing the correlation between the closure term and these three variables from one simulation dataset and then the transient of different initial conditions could be predicted using that correlation [3]. This statistical method may be applied to different cases without much insight into the physics.

Also, a novel approach was developed to utilize high fidelity simulation data by means of field inversion and machine learning [4]. Data are used to infer a functional form of the model discrepancy. This function is related to the low fidelity simulation using machine learning. The method was applied successfully to one dimensional heat conduction equation with convection and radiation sources to reconstruct the equation missing terms. It was also applied to turbulent channel flow problem to teach Reynolds averaged closure model given DNS data. Field inversion and machine learning approach has not been implemented in more complex problems. Factors like mesh size and numerical scheme weren't considered.

In our work, the major idea is to benefit from high fidelity simulation results to model the sub-grid effect in the CG-CFD. This approach aims to gain a surrogate model instead of the deterministic sub-grid scale model. We chose to start by a natural convection study as we already have a relevant validation matrix provided in [5]. The turbulent natural convection occurs in molten reactor core during a nuclear reactor accident and determines the thermal loading on reactor structural materials.

2. PROBLEM DESCRIPTION

We consider a natural convection case with volumetric heating in a horizontal fluid (water) layer with a rigid, insulated lower boundary, isothermal (cold) upper boundary (293K) and periodic boundaries at other sides, see Figure 1. The fluid layer is 2×2×2 inches and the volumetric heat generated is adjusted to get the desired Rayleigh number (9.3×10^7) which is defined as

$$Ra = \frac{g\beta H^5 q_v}{2k\nu\alpha} \tag{1}$$

Simulation is performed with CFD software, OpenFOAM [6], with a solver for buoyant, turbulent flow of incompressible fluids. The Boussinesq approximation is used so density changes due to buoyancy are incorporated in the body force only. Spalart-Allmaras model [7] (equations (6) and (7)) is applied to model turbulence (only for case when turbulence model is applied). Three-dimensional time-dependent governing equations of mass conservation (2), momentum conservation (3) and temperature (4) are solved with Boussinesq approximation (5):

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \tag{2}$$

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{u}_j\bar{u}_i\right) = -\frac{\partial}{\partial x_i}\left(\frac{\bar{p}}{\rho_0}\right) + \frac{1}{\rho_0}\frac{\partial}{\partial x_j}\left(\tau_{ij} + \tau_{t_{ij}}\right) + \frac{\bar{\rho}}{\rho_0}g_i \tag{3}$$

$$\frac{\partial \bar{T}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{u}_j\bar{T}\right) - \frac{\partial}{\partial x_k}\left(\left(\frac{\nu_0}{Pr} + \frac{\nu_t}{Pr_t}\right)\frac{\partial \bar{T}}{\partial x_k}\right) = \frac{q_v}{\rho C_p} \tag{4}$$

$$\rho_{eff} = 1 - \beta(T - T_0) \tag{5}$$

$$\frac{\partial \tilde{\nu}}{\partial t} + \bar{u}_j\frac{\delta\tilde{\nu}}{\partial x_j} = c_{b1}(1 - f_{t2})\tilde{S}\check{\nu} - \left[c_{w1}f_w - \frac{c_{b1}}{k^2}f_{t2}\right]\left(\frac{\check{\nu}}{d}\right)^2 + \frac{1}{\sigma}\left[\frac{\partial}{\partial x_j}\left((\nu + \check{\nu})\frac{\delta\tilde{\nu}}{\partial x_j}\right) + c_{b2}\frac{\delta\tilde{\nu}}{\partial x_i}\frac{\delta\tilde{\nu}}{\partial x_i}\right] \tag{6}$$

$$\nu_t = \check{\nu} f_{v1} \tag{7}$$

The initial velocity is set to zero and initial temperature is the upper wall temperature (293K). All three-dimensional calculations were performed using a grid similar to that used in [8] for direct numerical simulation of internally-heated unstably-stratified fluid layer (similar to present work). Mesh parameters are: $\Delta x/H = \Delta y/H = 0.029$, $\Delta z/H = 0.00096$. Based on Fourier moduli given in [8], time steps are chosen to be 1.8 seconds for Rayleigh number, 9.3×10^7.

We select the figure of merit (FOM) to be the temperature distribution through the fluid layer and the goal is to model the sub-grid effect in coarse-grained CFD to obtain sufficiently accurate prediction of FOM. This goal is achieved through the following steps:

- Fine mesh simulation is performed with the mesh parameters mentioned above. No turbulence model is used in the simulation.
- Fine mesh simulation is validated through comparing the Nusselt number and temperature distribution with those in [8] and [9].

- Coarse-grained simulation is conducted with Spalart-Allmaras turbulence model. Fluid layer coarse mesh temperature distribution is compared with that of fine meshes.
- A global correction is applied to the temperature equation, equation (4), by modifying the diffusion term as following:

$$\frac{\partial \bar{T}}{\partial t} + \frac{\partial}{\partial x_j}\left(\bar{u}_j \bar{T}\right) - \frac{\partial}{\partial x_k}\left(\left(\frac{\nu_0}{Pr} + \frac{\nu_t}{Pr_t} + \alpha_N\right)\frac{\partial \bar{T}}{\partial x_k}\right) = \frac{q_v}{\rho C_p} \tag{8}$$

  where α_N is an added diffusivity to compensate for the sub-grid error because of using a coarse mesh.
- A set of numerical experiments are performed to evaluate the range of values for α_N and to select the most suitable α_N.
- This process is repeated for different degrees of coarsening (different meshes) to develop a model for α_N.
- Analytical model for α_N is tested with a new case that has a different geometry (Fluid layer depth is modified).

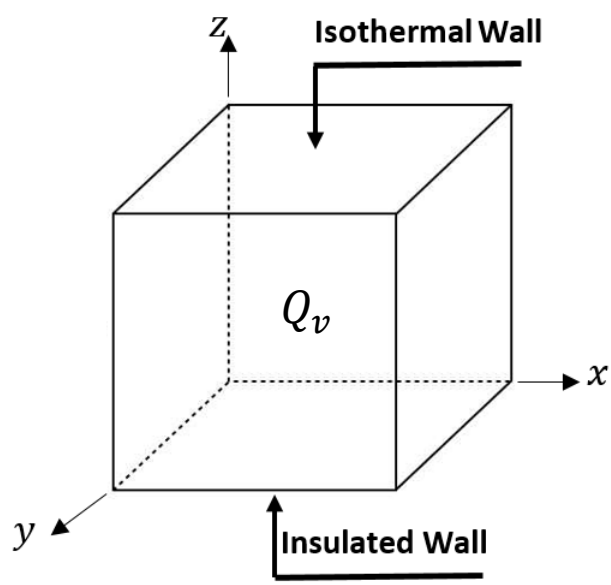

Figure 1. Computational domain with insulated lower boundary, isothermal upper boundary and periodic boundaries at other sides.

3. NUMERICAL RESULTS

A comparison between results of the current work and results of DNS simulation of turbulent natural convection at $Ra = 9.3 \times 10^7$in [8] is shown in Figure 2 and Figure 3. Temperature is averaged over 1000 time steps in the quasi-steady state region. In both figures, the results of both works agree fairly well. Figure 2 depicts the dimensionless temperature profile across the fluid layer. z/H is the normalized distance in the vertical direction along the axis of the fluid layer while $T^*$is the average dimensionless temperature, $T^* = 2k(T - T_w)/(q_v H^2)$. The temperature difference $(T - T_w)$ is normalized by $(q_v H^2/2k)$ which is

the maximum temperature difference that would exist in the fluid layer for purely conductive heat transfer [8].

In Figure 3, root mean square temperature fluctuations (in Kelvins) along the axis of the fluid layer is computed. It is noted that the maximum oscillation is found at the upper cooled surface. In [9], both igures 1 and 2 were validated against experimental data in [9]. It's worth noting that, the natural convection case presented in [7] is given in terms of Rayleigh number not fluid layer height so the comparison in terms of dimensionless numbers in Figure 2 is more consistent than that of Figure 3 where temperature fluctuations are given in Kelvins.

In Figure 4 and Figure 5, the comparison between the temperature profiles predicted by the high fidelity simulation vs. the profiles predicted by low fidelity simulation is presented. High fidelity simulation is done with a fine mesh (whose parameters are described before) without turbulence model while low fidelity simulation is performed with coarse meshes with 1-equation Spalart-Allmaras turbulence model. The time needed to get to the quasi steady state condition is around 1 hour, which is comparable to experimental work done before [8] (3-12 hours to get to steady state for a fluid layer whose height is 2-3 inches and width is 20 inches).

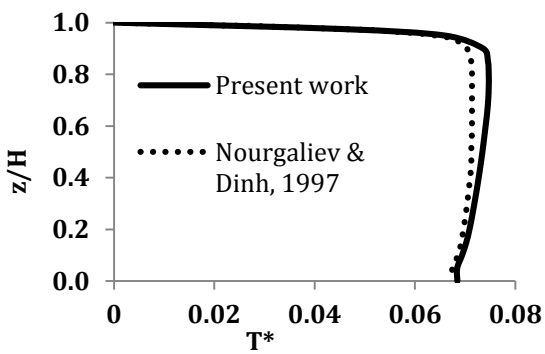

Figure 2. Temperature profile at $Ra = 9.3 \times 10^7$.

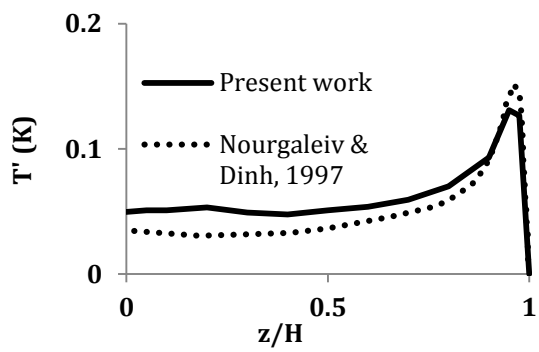

Figure 3. Temperature fluctuations at $Ra = 9.3 \times 10^7$.

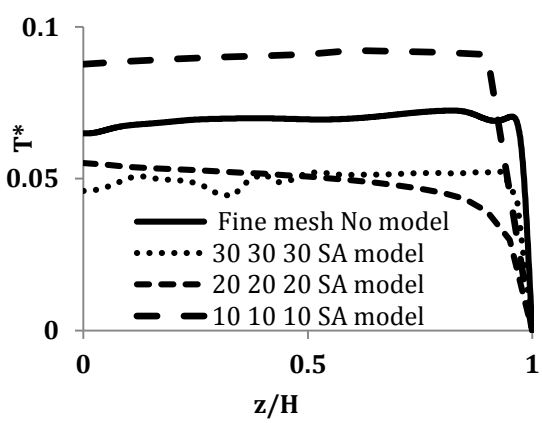

Figure 4. Temperature gradient at the vertical direction as computed with fine and coarse meshes at $Ra = 9.3 \times 10^7$.

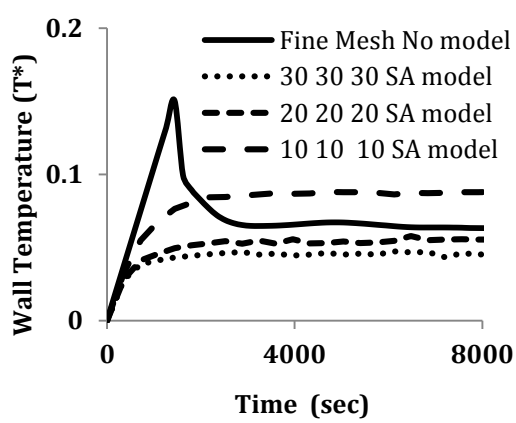

Figure 5. Insulated wall temperature change with time as computed with fine mesh and coarse meshes at $Ra = 9.3 \times 10^7$.

The insulated wall temperature behavior in Figure 5 may be attributed to the heat conduction and buoyancy forces. No heat flows from the insulated lower boundary while the fluid near the upper boundary is cooler and denser. Hence, heat is transferred by conduction in the beginning of the simulation. This leads to a temperature overshoot in the first 3000 seconds of the simulation. With increasing density variation, buoyancy force drives fluid motion so hot fluid near the lower boundary becomes less dense and rises. The cooler fluid replaces it and so on. Instability caused because of the competition between buoyancy force and cold boundary layer is shown in Figure 6.

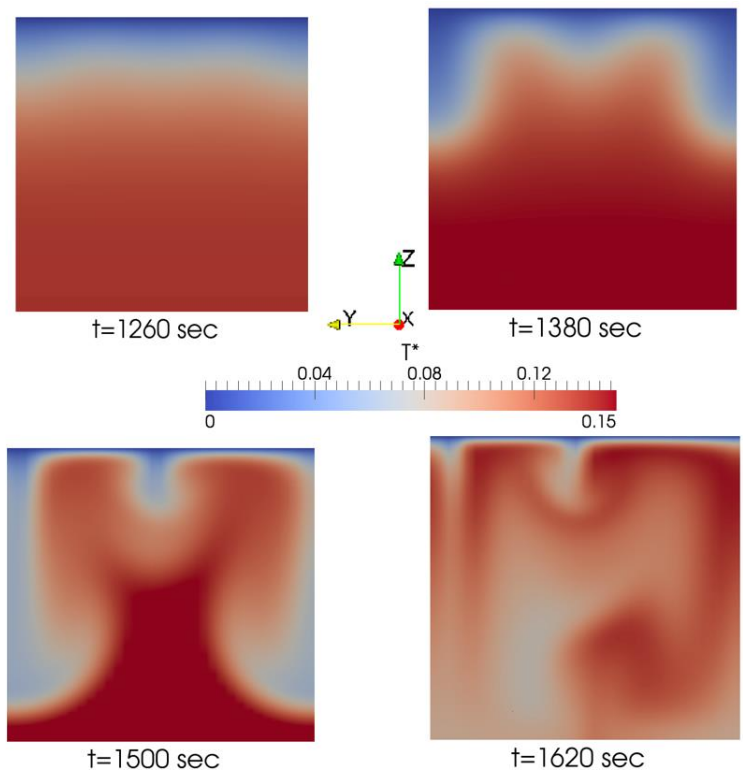

Figure 6. Example of calculated temperature field at different times. Temperature is given in dimensionless form, T*

Table 1 illustrates how simulation cost decreases with decreasing the mesh size starting from the fine mesh (in the first row) till the coarsest mesh, 10×10×10 nodes (in the last row). While the simulation performed with $10\times 10 \times 10$ nodes' mesh over-predict the temperature, the other coarse meshes under-predicted it. In Figure 5, the wall temperature (averaged over space) increases approximately linearly in the beginning of the simulation and then it decreases to get to quasi-steady state case after around 3000 seconds. Both fine mesh and coarse meshes simulation needed approximately the same stabilization period to get to a quasi-steady state.

Table 1. Simulation cost as performed by different meshes.

Mesh size (nodes)	Simulation cost (number of processors × number of hours)
1204552	61.7
27000	0.4
8000	0.1
1000	0.02

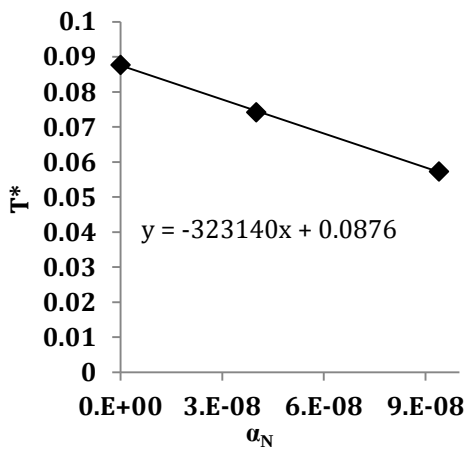

Figure 7. Adjusting α_N according to insulated bottom wall center temperature for 10×10×10 mesh.

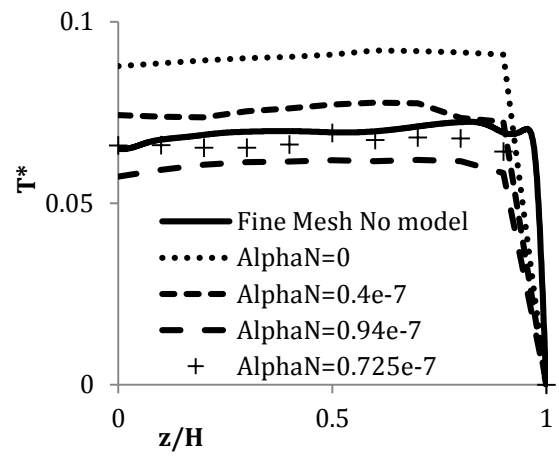

Figure 8. Comparison between axial temperature gradient as computed by fine mesh and coarse mesh (10×10×10) which is corrected by different values of α_N.

In order to improve the results predicted by the coarse mesh, the hypothesis we presented in equation (8) is tested as shown in the following figures. The parameter α_N is assigned an initial value and then, by doing numerical experiments, α_N can be adjusted to get approximately correct result with a coarse mesh. Figure 7 is an example of how α_N was adjusted to get the correct bottom wall center temperature ($T^* = 0.0659$) after three iterations.

In Figure 8, Figure 9 and Figure 10, it is shown how the vertical temperature profile (computed at the end of the simulation) was changed by changing the value of α_N. In each figure, the crossed line represents the best temperature profile we got by fixing α_N. Figure 11 shows the insulated wall temperature profile after being corrected by α_N. The temperature profile is corrected for the three coarse meshes but the transient predicted by the fine mesh simulation wasn't captured by any of the coarse mesh simulations. The correction by α_N impacted the temperature distribution throughout the whole fluid layer not the axial distribution only as presented in Table 2. In Table 2, both the average error and the maximum error for the temperature distribution at the end of the simulation, were reduced significantly after the correction. α_N, which is used to correct the results is plotted vs. the mesh size in Figure 12. Interestingly, the correction factor α_N changed approximately linearly with the mesh size which gives the capability to predict the correction needed with more mesh sizes. The linear equation is displayed in Figure 12 with the correlation coefficient squared, R^2.

A new case is designed with doubling the fluid layer height so the fluid layer is 4×4×4 inches. The Rayleigh number is maintained the same by changing the volumetric heat generated in the fluid. Fine mesh simulation is performed again with the same parameters mentioned before. Another simulation is done with a coarse mesh (10×10×10) with and without the correction by α_N. Here, α_N is the same of the mesh (10×10×10) of

2×2×2 inches case. In Figure 13, a comparison between the fine mesh simulation result and the coarse mesh simulation prediction (both corrected and non-corrected temperature profile) is illustrated .The correction, made to α_N, clearly improves the coarse mesh result for the new case.

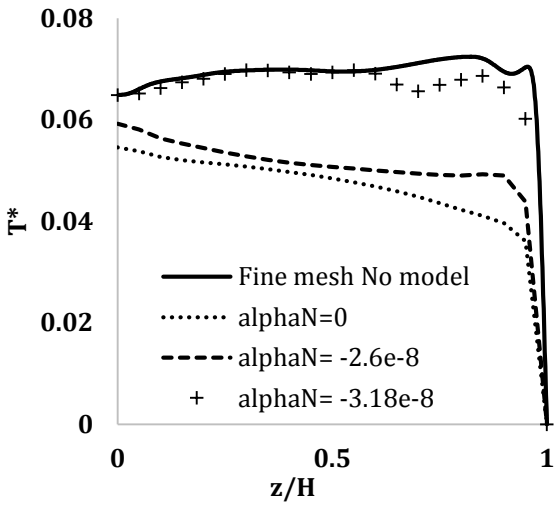

Figure 9. Comparison between axial temperature gradient as computed by fine mesh and coarse mesh (20×20×20) which is corrected by different values of α_N.

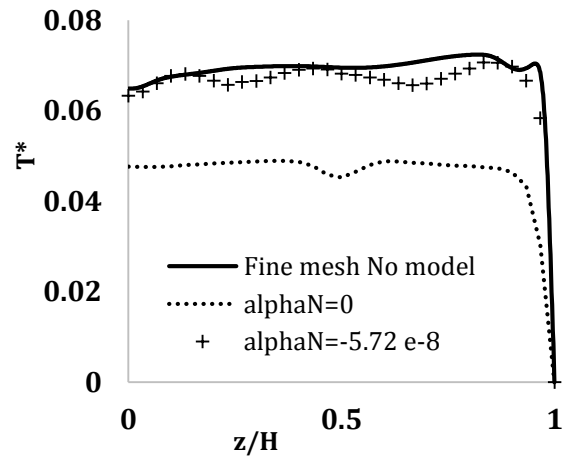

Figure 10. Comparison between axial temperature gradient as computed by fine mesh and coarse mesh (30×30×30) which is corrected by different values of α_N.

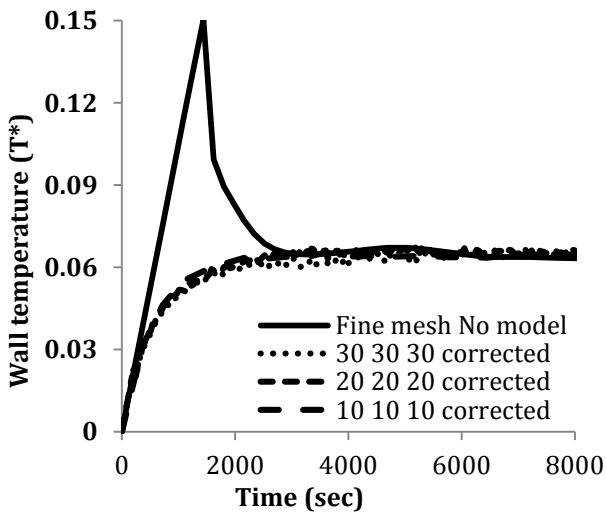

Figure 11. Comparison between insulated wall temperatures as computed by fine mesh and coarse meshes which are corrected by α_N.

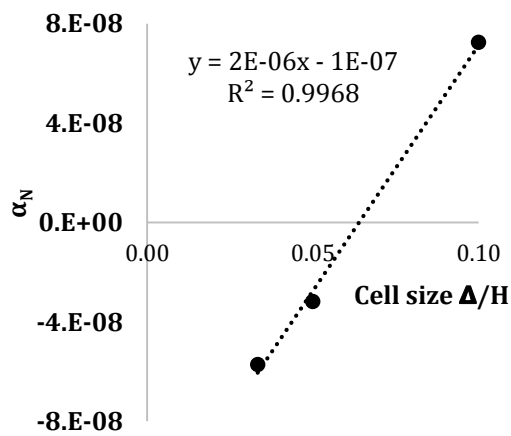

Figure 12. Variation of α_N with the mesh size.

Table 2. The error reduction occurred after correcting the coarse mesh (10×10×10) result with α_N.

Before correction average error	After correction average error	Before correction maximum error	After correction maximum error
32.2%	6.5%	79.1%	29.6%

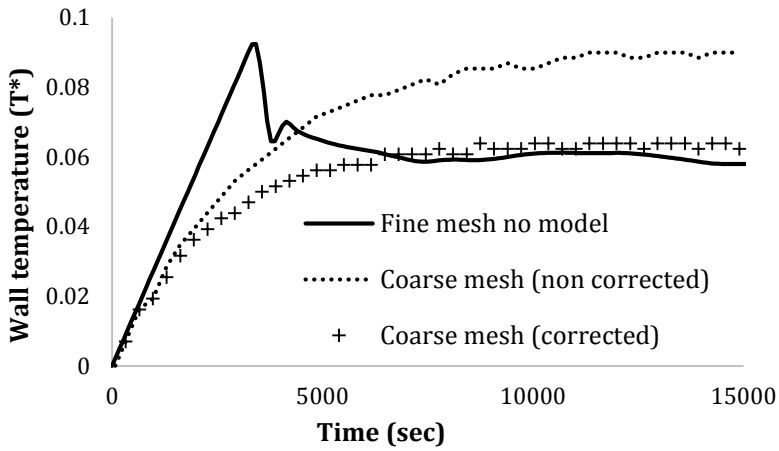

Figure 13. Comparison between insulated wall temperatures as computed by fine mesh and coarse mesh (10×10×10) which are corrected by α_N for a new case with double height.

4. CONCLUSIONS AND FUTURE WORK

Analysis of the turbulent natural convection case with volumetric heating in a horizontal fluid layer is performed with high fidelity simulation (with fine mesh) and lower fidelity 3D simulation (coarse mesh). The coarse mesh simulation was corrected by modifying the diffusion term in the energy equation. This global correction was presented as a function of the mesh size. The quasi-steady-state temperature distribution predicted with a coarse mesh is corrected without capturing the transient. We hypothesize that the same correction can be applied to different cases having the same Rayleigh number.

More work is needed to show the dependence of the corrected diffusivity on the Rayleigh number: in particular, the Rayleigh number may get to values as high as 10^{16} in the reactor case [8]. Additionally, it is important to investigate the dependence of the corrected diffusivity on fluid Prandtl number. Additional simulations are still needed to get a more complete library of state that gives the corrected diffusivity as a function of different fluids and different kinds of geometries (for example cube vs. hemisphere as well as more complex domains). Additionally, it would be more productive to get a correction parameter/function which is related to the local flow conditions, rather than to the global Rayleigh number.

NOMENCLATURE

Ra	Rayleigh Number	H	fluid layer height (m)
g	gravitational acceleration (m/s^2)	q_v	power generated per volume (W/m^3)
β	thermal expansion coefficient ($1/K$)	k	thermal conductivity ($W/(m.K)$)

ν	kinematic viscosity (m^2/s)
α	thermal diffusivity (m^2/s)
u	velocity (m/s)
T	temperature (K)
p	pressure (N/m^2)
$\mathbf{\Delta}$	spatial step (m)
T_w	upper wall fixed temperature
c_{b2}	$= 0.622$
σ	=0.67
c_{w3}	$= 2$
χ	$= \check{\nu}/\nu$
c_{t4}	$= 0.5$
W_{ij}	$= 0.5\left(\frac{\partial \overline{u_i}}{\partial x_j} - \frac{\partial \overline{u_j}}{\partial x_i}\right)$
d	The distance from the field point to the nearest wall.
f_{v1}	$= \frac{\chi^3}{\chi^3 + {c_{v1}}^3}$
$\tilde{S}$	$= \Omega + \frac{\check{\nu}}{k^2 d^2} f_{v2}$
f_w	$= g\left[\frac{1 + {c_{w3}}^6}{g^6 + {c_{w3}}^6}\right]^{1/6}$

ρ	density (kg/m^3)
τ_{ij}	stress tensor (N/m^2)
Pr	Prandtl number
ρ_{eff}	effective kinematic density
C_p	specific heat at constant pressure ($J/(kg.K)$)
c_{b1}	=0.1355
k	= 0.41
c_{w1}	$= \frac{c_{b1}}{k^2} + \frac{1 + c_{b2}}{\sigma}$
c_{t3}	$= 1.2$
f_{t2}	$= c_{t3} e^{-c_{t4}\chi^2}$
Ω	$= \sqrt{2W_{ij}W_{ij}}$
c_{v1}	$= 7.1$
c_{w2}	$= 0.3$
f_{v2}	$=1 - \frac{\chi}{1+\chi f_{v1}}$
r	$= min\left(\frac{\check{\nu}}{Sk^2d^2}, 10\right)$
g	$= r + c_{w2}(r^6 - r)$

Superscripts

*	dimensionless value
'	fluctuating component
‾	time-averaged value

Subscripts

0	reference value
t	turbulent component

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