Numerical Analysis of Algebraic Heat Flux Model in a Rectangular Cavity

Ralph Carlo Evidente, Seokwon Whang, and Hyun Sun Park*
Division of Advanced Nuclear Engineering, POSTECH, 77 Cheongam-Ro, Nam-Gu, Pohang 790-784, Gyeongbuk, Republic of Korea
*Corresponding author: heisunny@postech.ac.kr

1. Introduction

For the past decades, many researchers have been focusing in the area of severe accident in nuclear power plants, which has notable impacts in environment. One of its causes is long absence of the core cooling, which results to overheating and the possibility of relocation of melt pool to the lower plenum of reactor vessel. Corium, the molten mixture, can be stratified with a metallic layer coming from debris particles of reflector, steel, iron and zircaloy, above an oxide layer which is made up of ZrO₂ and UO₂. Heat transfer phenomena and fluid behavior in these layers play a vital role for the vessel integrity. One of which is natural convection involving internal heat source. The complexity of phenomena occurring inside the corium requires high-fidelity numerical simulation, as various CFD researchers take account into the wall modelling, constant eddy viscosity which can be modeled using Algebraic flux model (AFM) from Equation 5 to 8 [4,5], and heat flux parameters. Many experiments involving turbulent natural convection phenomena have been used to validate against the simulation results. One of these [1] took account of natural convection boundary layer in a rectangular cavity filled with air and having an aspect ratio of five. Numerical validation involving this experimental study generally uses RANS turbulence models to estimate flow details and local heat transfer for complex flows. Meanwhile, turbulent heat flux in general is calculated using either SGDH, GGDH, or AFM depending on various circumstances.

Simulation results using Simple Gradient Diffusion Hypothesis (SGDH) have been reported to yield inaccurate solutions for natural convective flows. Meanwhile, General Gradient Diffusion Hypothesis (GGDH) is used for conditions involving shear dominant flows, but not for strongly stratified natural convective flows [2]. Algebraic flux model may require another transport equation, but it has been proven pragmatic for buoyancy-driven and stratified flow conditions. Many CFD researchers [3] have still reported that convergence using advanced models were hardly achievable, and hence a further study is necessary. The objectives of this study are to implement algebraic flux model (AFM) in the chosen CFD solver, validate it against the experimental data, and depict its flow behavior using global, turbulent, and heat flux parameters.

2. Methodology

The analysis of the turbulent natural convection is mathematically described by the equations of conservation of mass, energy, and momentum. RANS methodology is utilized for solving these equations involving incompressible buoyancy-driven flow. Assuming Boussinesq approximation, governing equations for this study are

\[
\frac{\partial U_i}{\partial t} + \frac{\partial}{\partial x_j} \left( U_i U_j \right) = - \frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j} \left( \nu \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} \right) - \frac{2}{3} \kappa \delta_{ij} \]

in which, \( U_i \) is a component of mean velocity and \( T \) is the mean temperature. Both the turbulent stress, \( \overline{u_i u_j} \), and turbulent heat flux, \( \overline{\theta u_i} \), represent the unresolved turbulence contributions, which need to be modeled to close the above equations.

The turbulent stress, \( \overline{u_i u_j} \), was given by the Boussinesq hypothesis as follows:

\[
\overline{u_i u_j} = \nu_T \frac{\partial U_i}{\partial x_j} + \frac{2}{3} \kappa \delta_{ij}
\]

where \( k \) is the turbulence kinetic energy and \( \nu_T \) is the eddy viscosity which can be modeled using \( \omega \)-omega shear stress (SST) transport equations. The latter has proven to capture physics phenomena near and away from the wall because of its blending function.

On the other hand, turbulent heat flux \( \overline{\theta u_i} \) in this study will be modeled using AFM from Equation 5 to 8 [4,5]:

\[
\overline{\theta u_i} = -C_v \frac{k}{\varepsilon} \left( C_1 \overline{u_i u_j} \frac{\partial T}{\partial x_j} + C_2 \overline{\theta u_i} \frac{\partial U_j}{\partial x_j} + C_3 \beta g_i \right)
\]

\[
\frac{\partial \overline{\theta^2}}{\partial t} + U_j \frac{\partial \overline{\theta^2}}{\partial x_j} = \frac{2\nu_T \overline{\theta u_j}}{\sigma_{\theta^2}} \frac{\partial \overline{\theta^2}}{\partial x_j} + \frac{\partial}{\partial x_j} \left[ u_i \frac{\partial \overline{\theta^2}}{\partial x_j} \right]
\]

\[
\varepsilon_\theta = \frac{\varepsilon \overline{\theta^2}}{2Rk}
\]
\[ R = \frac{\tau_{th}}{\tau_m} \approx 0.5 \]  

where \( \theta^2 \) is the temperature variance, \( \varepsilon_\theta \) is its dissipation, and \( R \) as the thermal-to-mechanical time-scale ratio.

In this study, coefficients used in AFM equations [5] (Table 1) will be adopted from the reference [4]. The behavior from AFM computations will also be compared along with the standard approaches seen on Table 2.

**Table 1**: Coefficients Adopted from this study

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>C_0</th>
<th>C_1</th>
<th>C_2</th>
<th>C_3</th>
<th>C_4</th>
</tr>
</thead>
<tbody>
<tr>
<td>Air</td>
<td>0.15</td>
<td>0.6</td>
<td>0.6</td>
<td>0.6</td>
<td>1.5</td>
</tr>
</tbody>
</table>

**Table 2**: Treatment of Turbulent Heat Flux [5]

<table>
<thead>
<tr>
<th>Approach</th>
<th>Equations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Simple Gradient</td>
<td>( \overline{\theta u_i} = \frac{-\nu_r \partial T}{P r_T \partial x_i} )</td>
</tr>
<tr>
<td>Diffusion Hypothesis (SGDH)</td>
<td></td>
</tr>
<tr>
<td>General Gradient</td>
<td>( \overline{\theta u_i} = -C_0 \frac{k}{\varepsilon} (u_j u_j) \frac{\partial T}{\partial x} )</td>
</tr>
<tr>
<td>Diffusion Hypothesis (GGDH)</td>
<td></td>
</tr>
</tbody>
</table>

In this study, coefficients used in AFM equations [5] (Table 1) will be adopted from the reference [4]. The behavior from AFM computations will also be compared along with the standard approaches seen on Table 2.

**Table 3**: Initial and Boundary Conditions

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Initial condition</th>
</tr>
</thead>
<tbody>
<tr>
<td>DHC</td>
<td>Air</td>
</tr>
<tr>
<td>Ra</td>
<td>5.2 x 10^{10}</td>
</tr>
<tr>
<td>Gr</td>
<td>7.4 x 10^{10}</td>
</tr>
<tr>
<td>( \frac{T_{hot}}{T_{cold}} ) (dT)</td>
<td>339.15K/295.35K (43.8K)</td>
</tr>
<tr>
<td>\nu</td>
<td>1.73 x 10^{-5}</td>
</tr>
<tr>
<td>\beta</td>
<td>3.15 x 10^{-3}</td>
</tr>
<tr>
<td>Pr</td>
<td>0.7</td>
</tr>
<tr>
<td>No slip-condition</td>
<td>( u_i = 0 )</td>
</tr>
<tr>
<td>Reynolds stress</td>
<td>( u_i u_j = 0 )</td>
</tr>
<tr>
<td>Turbulent heat flux</td>
<td>( \frac{\theta}{\theta} = 0 )</td>
</tr>
<tr>
<td>Temperature</td>
<td>( \frac{\theta}{\theta} = 0 )</td>
</tr>
<tr>
<td>Dissipation</td>
<td>( \varepsilon = 2\nu k / \gamma^2 )</td>
</tr>
</tbody>
</table>

**Fig. 1**: Geometrical Configuration

A 2-D rectangular cavity with an aspect ratio of 5:1, as well as its boundary condition, can be seen in Fig.1. Other numerical parameters for initial condition and constant values used in this study can be seen in Table 3 and are implemented in OpenFOAM CFD software. A maximum dimensionless height value (y^*) of 4.5 can be seen in Fig.2., which is measured along the hot wall. The generated graph was based on the mesh geometry, and it is in accordance of recommended dimensionless height values for SST-based models.

**Fig. 2**: Dimensionless height generated from mesh

3. Results and Discussion

AFM is plotted against the standard cases. SST plot is solved using buoyantBoussinesqSimpleFoam OF solver, and is included solely for validation purposes against the results from SGDH-implemented simulation. Likewise, GGDH and AFM are both implemented based on the equations from the reference [5]. Contour resulting images for global parameters that can be seen in Fig. 3 are well-matched with the temperature and velocity profile in Fig.4a and 4b. Edged-like peak behavior is apparent for the vertical velocity profile (Fig.4a). The significant differences can be seen starting from the peak until before the plots get dampened. GGDH and AFM lie at the same apex; on the other hand, SGDH yielded the maximum point. All case models over-predicted the experimental data. For temperature profile, AFM is noticeable among other cases as depicted below and above of the theoretical mean temperature line. Regarding the experimental plots of turbulence parameters (i.e. turbulent kinetic energy and Reynolds shear stress), it was reported very hard to establish a perfectly insulated boundary in the experiment.
and thus generated asymmetric flows [3]. It was partly because of imperfect insulation at the ceiling of the cavity where the small amount of heat loss prohibits the flow from relaminarization; hence, the latter took place at the bottom of cavity. The simulation results showed that AFM are under-predicted by other case models. Distinguished gaps can be observed starting from the peak until its dampening behavior, with AFM gave the higher values followed by SGDH and GGDH, respectively. Meanwhile, as seen in Fig. 5, sharp edged peaks in the generated THF plots, despite using high resolution, are depicted in the maxima behavior of all cases. Similar tendency is observed for AFM and SGDH for the horizontal turbulent heat flux, while AFM produced maximum peak for vertical turbulent heat flux, similar to previous studies [4]. If one would zoom in the plot of vertical THF, AFM gives hollow-like minima behavior before it reaches to the center of midwidth.

**Fig. 3:** Contour Plots with (left) velocity and (right) temperature

**Fig. 4:** (a) Velocity, (b) Temperature, (c) Turbulent Kinetic energy, and (d.) Reynolds Shear Stress measured through the midwidth (y/H = 1.25) of the cavity
4. Conclusion

Using OpenFOAM 2.3, a validation study was conducted as it plays a vital role in the turbulent heat flux (THF) implementation before proceeding to numerical analysis involving turbulent natural convection phenomena of oxide layer of corium pool. Transport equations of THF were implemented in the CFD solver, and their results were validated against the experimental data. Several parameters were used to observe the differences among the turbulent heat flux models, namely: (1) global parameters (vertical velocity and temperature), (2) turbulence parameters (turbulent kinetic energy and Reynolds shear stress), and lastly (3) vertical and horizontal turbulent heat fluxes. Based on the generated plots, convergence is still hardly achievable for AFM; hence, a grid convergence and sensitivity analyses have to be properly assessed.

With proper generated mesh geometry, one can avoid the peak issue uncertainties, as it will pave the way to correctly depict the turbulent thermal behavior in the boundary near-wall region. Moreover, several CFD researchers have attempted to modify the AFM equations. The equation that this study used is more notably known as AFM-2005 equation. It was originally developed for natural convection flow regime for unity Prandtl fluids. Meanwhile, for non-unity Prandtl fluids and for different flow regimes, a modification was done by previous studies to calibrate $C_{1}$ and $C_{3}$ as these give sensitivity in scenarios involving forced convection and natural convection, respectively.

Currently, a follow-up simulation is being conducted to assess the sensitivity analysis using wide range of coefficient values with the same conditions implemented in differential heated cavity case, and thus will be presented in the upcoming Autumn meeting.

Acknowledgement

This work was supported by KOREA HYDRO & NUCLEAR POWER CO., LTD. This work was supported by KOREA HYDRO & NUCLEAR POWER CO., LTD (No. Safety 2-1, “High-Fidelity Numerical Analysis of Highly Turbulent Corium Pool for In-Vessel Retention (IVR) Strategy Feasibility Assessment”)

REFERENCES