**LES SOFTWARE FOR THE DESIGN OF LOW EMISSION COMBUSTION SYSTEMS
FOR VISION 21 PLANTS**

Quarterly Technical Progress Report for

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by

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ABSTRACT

Previous LES calculations for one SIMVAL case ($\phi_{inj} = 0.7$) have repeatedly shown that the heat transfer/heat losses were not correctly captured, resulting in predicted NO_x emissions being much higher than measurements. In a current Navy Phase I SBIR project, we are studying ways to improve the prediction of heat transfer/heat loss in LES calculations. To improve our understanding of heat transfer at walls, a series of thermal channel flow cases were analyzed and compared to DNS predictions. When trying to fully resolve the boundary layer, it was found that the grid size in all directions (i.e. Δx , Δy , and Δz) must be smaller than the size of eddies formed in the boundary layer. Thus, the cell aspect ratio at the wall needs to typically be less than 25 when the boundary layer is being resolved. In previous SIMVAL LES calculations, this cell aspect ratio requirement was not followed, and thus the heat transfer was less than desired. For this quarter, the grid was adjusted, and the SIMVAL case was rerun. The LES results show that vortices are now formed in the exhaust duct near the walls, resulting in more heat loss from the exhaust duct flow and lower NO_x predictions (more in line with the measurements).

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1. INTRODUCTION

Vision 21 combustion systems will require innovative low emission designs and low development costs if Vision 21 goals are to be realized. In this three-year project, an advanced computational software tool will be developed for the design of low emission combustion systems required for Vision 21 clean energy plants. The combustion Large Eddy Simulation (LES) software will be able to accurately simulate the highly transient nature of gaseous-fueled turbulent combustion so that innovative concepts can be assessed and developed with fewer high-cost experimental tests. During the first year, the project included the development and implementation of improved chemistry (reduced GRI mechanism), subgrid turbulence (localized dynamic), and subgrid combustion-turbulence interaction (Linear Eddy) models into the CFD-ACE+ code. University expertise (Georgia Tech and UC Berkeley) was utilized to help develop and implement these advanced submodels into the unstructured, parallel CFD flow solver, CFD-ACE+. Efficient numerical algorithms that rely on *in situ* look-up tables or artificial neural networks were implemented for chemistry calculations. In the second year, the combustion LES software was evaluated and validated using experimental data from lab-scale and industrial test configurations. This code testing (i.e., alpha testing) was performed by CFD Research Corporation's engineers. During the third year, six industrial and academic partners used the combustion LES code and exercised it on problems of their choice (i.e., beta testing). Final feedback and optimizations were then be implemented in the final release version of the combustion LES software that will be licensed to the general public.

An additional one-year task was added for the fourth year of this program entitled, "LES Simulations of SIMVAL Results." For this task, CFDRC will perform LES calculations of selected SIMVAL cases, and compare predictions with measurements. In addition to comparisons with NO_x and CO exit measurements, comparisons will be made to measured pressure oscillations. Possible gaps in the data sets will be identified, as well as potential areas of improvement for combustion and turbulence models.

2. EXECUTIVE SUMMARY

Work in this fourteenth quarter (January – March 2004) has included further validation of the LES software with SIMVAL experiments. Improved agreement between predictions and measurements has been achieved by modifying the near-wall grid to resolve turbulent eddies. Additional cases will be run next quarter.

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS

4.1 Thermal Channel Flow Analysis

Under a Navy Phase I SBIR project, CFDRC studied flow within a heated channel to determine the effects of grid spacing on turbulence and heat transfer. The geometry and grid of the baseline case are shown in Figure 1. The channel was periodic (flow discharging the exit of the domain was input at the inlet of the domain) in both the streamwise and crosswise directions. Walls were located on the top and bottom of the channel. The channel was 3.5 m long, 0.42 m wide, and 0.56 m high. The baseline grid had 100,000 cells, and fully resolved the boundary layers ($y^+ < 1$ in first cell). The Reynolds number of this case was 3000 based on channel half height. The top wall was set at a temperature of 400K, and the bottom wall set at a temperature of 300K. DNS data from Debusschere and Rutland (2003) were available for comparison with our LES calculations.

Snapshots of the V-velocity (for reference, the flow velocity was U-velocity) and temperature are shown in Figure 2. The individual eddies are well captured by the LES calculation, in which the Localized Dynamic Kinetic energy Model (LDKM) was used for subgrid turbulence. Comparison of time-averaged axial velocities and temperatures against DNS data are shown in Figure 3 along the channel height. It can be seen that the LES predictions match well with the DNS data. Please note that these calculations fully resolved the boundary layers.

During the course of our study, we uncovered that certain grids, that seemed quite fine, produced purely laminar flows at the same conditions. For instance, if the grid shown in Figure 1 (with a $y^+ < 1$) was modified in the x direction only (removing every other grid line), a laminar solution was obtained. To capture the near wall eddies, all near wall grid dimensions (Δx , Δy , and Δz) must be small enough to capture the eddies. This finding means wall cell aspect ratios of 25 or less are required for LES calculations that fully resolve the boundary layer.

Unfortunately, it is unrealistic (in a computational sense) to fully resolve boundary layers in practical LES simulations of more complex geometries (such as the SIMVAL combustor). Instead, LES wall function models are needed, both for velocities and energy, so that grids with $y^+ \sim 25$ at the wall can be used. For velocity wall functions, a preliminary version of the Turbulent Boundary Layer Equation (TBLE) outlined by Wang and Moin (2002) was implemented into the LES software, as discussed below.

Figure 1. Channel Geometry Showing LES Grid that Fully Resolves Boundary Layers

Figure 2. Velocity (Top) and Temperature (Bottom) Snapshot Contours in Thermal Channel Flow Simulation

Figure 3. Comparison of Velocity and Temperature Profiles for a LES Calculation (Fully Resolved Boundary Layer) and DNS Data

In the TBLE model, the wall normal velocity is set to zero at the wall and the following equation is solved in the direction of the flow velocity tangential to the wall.

$$\frac{\partial}{\partial x_2}(\nu + \nu_t) \frac{\partial u_i}{\partial x_2} = F_i, \quad F_i = \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} u_i u_j. \quad (1)$$

In Equation 1, the eddy viscosity ν_t can be obtained using one of several mixing-length eddy viscosity models. The following model has been used in the implementation in CFD-ACE+

$$\frac{\nu_t}{\nu} = \kappa y_w^+ \left(1 - e^{-y_w^+/A} \right)^2. \quad (2)$$

The TBLE equation is solved numerically at each wall cell using a numerical 1-D domain spaced uniformly between the wall the center of the first computational cell. Due to the complexity of solving for and storing the velocity gradients needed to compute the last two terms in Equation 2, a simplified form of the TBLE model is currently being used in CFD-ACE+. The simplified approach drops the time-dependent velocity and velocity gradient terms. The pressure gradient term is still included in the model. Using this assumption, Equation 1 reduces to an ordinary differential equation that can be easily integrated numerically to calculate the wall shear stress. The full TBLE model will be implemented during Phase II of the Navy SBIR Program.

To show the need for improved LES wall functions, additional LES calculations of the thermal channel flow were performed with an y^+ of approximately 20. The preliminary TBLE model was used for near-wall velocity, and the highly-inaccurate Reynolds analogy was used for near-wall energy. LES predictions for velocity and temperature across the channel height are compared with the DNS data in Figure 4. It can be seen that improvements are needed, and will be addressed in Phase II of the Navy SBIR (if awarded).

Figure 4. Comparison of Velocity and Temperature Profiles for LES (Wall Function Treatment) Versus DNS Data

4.2 Latest SIMVAL Predictions

The grid of the last SIMVAL case (reported in the last quarterly) was assessed, and it was found that the near wall grid had aspect ratios ($\Delta x/\Delta y$) greater than 25. Thus, although the near wall y grid dimensions produced a y^+ of 1, the grid was too coarse in the axial direction, causing the flow to laminarize next to the wall. Rather than making the grid finer in the axial direction (and fully resolving the boundary layer), we made the grid coarser in the radial (y) dimension, thus producing a grid with y^+ around 20, and keeping the near wall aspect ratios around 1-2. We used LES wall functions for velocity and energy as described previously (recognizing their inadequacies that will be addressed in the future). Snapshots of temperature and NO_x of the current LES calculation (see Figures 5 and 6) show the improvement in the predictions now that vortices near the wall are being captured. Note the vortices captured at the entrance to the exhaust duct and extending downstream. For comparison, temperature and NO_x snapshots of the calculation reported in the last quarterly are also shown in Figures 5 and 6, and the lack of vortices in the exhaust duct is evident for the previous calculation. Also note that NO_x was not formed in the exhaust duct in the recent simulation, while it was formed in the previous simulation.

As has been mentioned in previous quarterlies, the LES predictions to date have not correctly predicted heat loss, and thus NO_x has been overpredicted. It now seems that part of the inaccuracy is the result of the near-wall grid having too large of an aspect ratio, resulting in laminar heat transfer coefficients at the walls, and no way to spread the heat loss through the flowfield (i.e. laminarization of the near-wall flow). One solution to this dilemma is to fully resolve the boundary layer, but this is too impractical. Therefore, we are taking the approach of developing LES wall function models, and using grids that do not fully resolve the boundary layers. Although a number of researchers are looking at LES wall function models for velocities, there does not appear to be anyone looking at LES wall function models for energy. This is an area needing future funding support.

Figure 5. LES Temperature Snapshots

Figure 6. LES NO_x Snapshots

5. REFERENCES

- Debusschere, B. and Rutland, C.J., (2003), "Turbulent Scalar Transport Mechanisms in Plane Channel and Couette Flows," *International Journal of Heat and Mass Transfer*, Vol. 47, pp. 1771-1781
- Wang, M. and Moin, P., (2002), "Dynamic Wall Modeling for Large-Eddy Simulation of Complex Turbulent Flows," *Physics of Fluids*, Vol. 14, pp. 2043-2051.

APPENDIX A — WORK SCHEDULE

Key Milestones

- 1 Complete In-Situ Adaptive Tabulation Module
- 2 Complete LES Framework Modification to CFD-ACE+
- 3 Complete Reduced Mechanisms
- 4 Complete Selection of Cases
- 5 Complete Implementation of Turbulence Models
- 6 Complete Implementation of Initial Version of LEM Model

- 7 Complete Tabulation Schemes
- 8 Complete Parallelization of LES Code
- 9 Complete Implementation of LEM Model
- 10 Complete Alpha Testing of LES Code
- 11 Complete Beta Testing of LES Code
- 12 Final Release of LES Code
- 13 Complete SimVal Comparisons

Performance Targets

- A Alpha Release of LES Code
- B Beta Release of LES Code
- C Final Commercial Release of LES Code

- Planned
- Performed

APPENDIX B — FUTURE PLANS

Additional SIMVAL cases will be analyzed with the combustion LES software, including parametric analyses with different ϕ_{inj} . Expectations are that the combustion pressure dynamics will be well captured by the simulations, and the cause of the sudden increase of dynamics at $\phi_{inj} = 0.6$ will be explained.