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

Quarterly Technical Progress Report for

July – September 2004

by

**Karl V. Meredith
Clifford E. Smith**

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**Technical Monitor: Mr. Norman T. Holcombe
Contract Monitor: Ms. Crystal Sharp**

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ABSTRACT

Work in this quarter focused on the continued running of two SIMVAL cases: ϕ (equivalence ratio) of 1) 0.55 and 2) 0.625. Comparisons were made between RANS and LES predictions for the ϕ of 0.625 case. The LES calculation showed a different flow pattern in the combustor compared to the RANS calculation, in particular the combustor recirculation flow pattern on the centerline is dramatically different. To demonstrate that the LES solution is accurate (and the RANS is not), non-reacting cases based on the Lilley experiment (Lilley, 1985) were run. Results from the Lilley cases verified that the LES calculations more closely match experimental velocity measurements for highly swirled, turbulent flows with a downstream constriction. In particular, RANS predictions show a strong centerline recirculation zone in the combustor, while LES predictions show positive axial velocity on the centerline, and an annular recirculation zone around the centerline.

Animation files were also created this quarter, so as to better demonstrate the LES predictions.

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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 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 sixteenth quarter (July – September 2004) has included further validation of the LES software with SIMVAL experiments completed in June, 2004. The LES predictions of combustion dynamics were lower than the measurements, although the LES calculations probably need longer run times before this conclusion can be definitely stated.

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS

Snapshots of u-velocity and temperature are shown in Figure 1 for the ϕ of 0.625 case. The snapshots show small features and flow unsteadiness, including vortices in the shear layers and vortices next to the wall in the exhaust duct. Comparison of time-averaged LES velocity predictions (u-velocity and w-velocity) and RANS velocity predictions are presented in Figure 2. It is evident that the LES-predicted flowfield is dramatically different than the RANS-predicted flowfield. RANS predicts a large, central recirculation zone on the centerline, while LES predicts positive axial velocity on the centerline and an annular recirculation zone. The LES solution also has distinct differences in the exhaust duct, including a lower velocity on the centerline than the RANS solution. The swirl velocity in LES is much higher in the premix passage than the RANS swirl velocity (although both solutions have the same inlet swirl velocity). The swirl velocity in LES is also much higher in the combustor, entering the exhaust duct, and in the exhaust duct.

Figure 3 presents comparison of temperature contours for RANS and time-averaged LES. The average temperatures are nearly the same, although the LES calculation shows some flame on the inner diameter of the centerbody (premix passage exit), while the RANS calculation does not. The NO_x comparisons show a dramatic difference between LES and RANS, caused by the difference in residence times. The RANS solution predicts most of the NO_x is formed in the central recirculation zone, and little NO_x is formed in the exhaust duct. In contrast, LES predicts little NO_x formed in the combustor, and a substantial amount of NO_x formed in the exhaust duct. Overall, the LES NO_x at the exhaust exit was 9.5 ppm, while the RANS NO_x was 7.0 ppm. Comparison to SIMVAL measurements, presented in Figure 4, shows the LES predictions to be in better agreement with the measurements.

Predictions of combustion dynamics are shown in Figure 5 for the two equivalence ratio cases. LES predicts a relatively quiet flame, and two dominant frequencies: 400 Hertz and 1300 Hertz. The predicted rms pressure levels are lower than the measurements (see Figure 6). Longer run times may be required in the LES calculations.

A number of animations of the ϕ of 0.625 case was performed. The starting frames of these animations are shown in Figures 7 and 8. These animations will be useful in demonstrating and understanding the unsteadiness of the flowfield.

In addition to modeling the SIMVAL experiment, two additional cases were analyzed to help understand the different turbulent, swirling flowfields being predicted by RANS and LES. The experiment of Lilley, 1985, was analyzed. The Lilley geometry was very similar to the DOE SIMVAL geometry, including an annular swirler, a centerbody, a dump combustor, and constriction downstream of the combustor. The cases selected for analysis had 45 degrees swirlers, a dump ratio (d/D) of 2.0, a combustor length of 2D, and a contraction nozzle with an area ratio of four. Two other swirl cases were experimentally tested: zero degrees and 70 degrees. Artistic impressions of dividing streamlines with and without contraction nozzle are shown in Figure 9 (from Lilley, 1985). It can be seen that the contraction nozzle had a strong effect on the centerline recirculation zone, resulting in an annular recirculation zone and positive axial velocity on the centerline.

The 45 degree swirler cases with and without contraction nozzle were analyzed using RANS and LES. The predictions are shown in Figure 10. It can be seen that LES captures the annular recirculation zone for the contraction nozzle case, while RANS does not. This is a very important finding, and shows the need of developing LES codes for improved mixing predictions.

5. REFERENCE

Lilley, D.G., (1985), "Swirling Flows in Typical Combustor Geometries," AIAA-85-0184, AIAA 23rd Aerospace Sciences Meeting, Reno, NV.

$$\phi = 0.625, \quad T_3 = 600 \text{ K}, \quad P_3 \approx 75 \text{ psia}$$

Figure 1. Velocity and Temperature Snapshots from Recent 3D LES Results

Figure 2. Comparison of Velocity Predictions for RANS and LES

Figure 3. Comparison of Temperature and NO_x Predictions for RANS and LES

Figure 4. Comparison of NO_x Predictions with SIMVAL Measurements

Pressure (Pa)
Trace

RMS
Pressure (Pa)

Figure 5. Predicted LES Combustion Dynamics

Figure 6. Comparison of Predicted LES Combustion Dynamics with SIMVAL Measurements

Figure 7. Initial Snapshots of Temperature Animations

Figure 8. Initial Snapshots of Velocity and NO_x Animations

Figure 9. Artistic Impression of Dividing Streamlines from Lilley Experiment

Without Contraction Nozzle

Figure 10. RANS and LES Predictions of Lilley 45 Degree Swirler Case (Without Contraction Nozzle)

With Contraction Nozzle

Figure 10 (cont). RANS and LES Predictions of Lilley 45 Degree Swirler Cases (With Contraction Nozzle)

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

The final report will be written during the next quarter and submitted to DOE.