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

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**by**

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## ABSTRACT

The new combustion Large Eddy Simulation (LES) code developed previously in this project was modified in two ways: 1) an improved inlet boundary condition for turbulence was implemented and 2) a new formulation for the variance (fluctuation) of progress/mixture fraction variables used in the assumed pdf turbulence-combustion interaction subgrid model was implemented. These code modifications were performed under a separate Navy Phase II SBIR and are briefly discussed in this DOE quarterly report for completeness. After these modifications were tested and verified, one SIMVAL case ($\phi_{inj}$=0.7) was run and predictions compared to SIMVAL data. The new LES calculation showed that the flame anchored at the correct location on the premix tube centerbody (in previous cases, the flame was incorrectly anchored just downstream of the swirler). The inlet turbulence effects resulted in more fine-scale structure being captured by LES, more-in-line with what we expected in LES calculations. The predicted $NO_x$ emissions were much higher than measurements, but it was realized that the heat losses throughout the combustion section and exhaust duct were lower than measured. The case will be rerun with the correct heat loss. The predicted pressure dynamics agreed well with the extrapolated measurements, although the case analyzed ($\phi_{inj}$=0.7) was not the best case to assess combustion dynamics. Additional cases are being run at $\phi_{inj}$ of 0.6 and 0.65 to assess our ability to correctly predict pressure dynamics.

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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 case, 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 thirteenth quarter (October - December 2003) has included further validation of the LES software with SIMVAL experiments. Improved agreement between predictions and measurements has been achieved by incorporating two code modifications. Additional cases will be run next quarter.

# 3. EXPERIMENTAL

No experiments were performed this quarter.

## 4. RESULTS

### 4.1 Multi-Step PDF Model with Dynamic $C_\varepsilon$

Under a Navy Phase II SBIR program, CFDRC developed and implemented a dynamic model of the mixture fraction variance (applicable to the progress variable variance as well) named the Localized Dynamic subgrid Variance Model (LDVM). This model is necessary for the use of the assumed PDF methodology to account for turbulence-chemistry interactions with LES. Previous simulations have shown that the scalar dissipation model coefficient $C_\varepsilon$ varies significantly in LES calculations for premixed flames. A new, innovative procedure for calculating this coefficient in a dynamic manner was conceived and implemented.

### 4.2 Improved LES Inflow Boundary Conditions

One significant problem encountered in LES modeling of turbulent flow is the specification of the inflow boundary conditions. For simulations that inherently generate a great deal of turbulence, specification of the inflow boundary condition turbulence levels is not that critical, as the flow will generate its own turbulence. However, to capture flow features that depend on the free-stream turbulence, such as flow separation and boundary layer transition, improved boundary conditions are needed. The standard approach is to specify a random inlet condition for each time to give the right values of turbulent fluctuations based on some estimated turbulent kinetic energy. This is the traditional, and simplest way, to handle specification of turbulent energy at the inlet boundary condition. However, the structures introduced with this approach are small scale (on the order of the grid size) and tend to dissipate very quickly, with the end result being nearly identical to a laminar flow boundary. Over the past quarter under a Navy Phase II SBIR program, several improvements to the LES modeling capabilities with respect to inlet boundary conditions in CFD-ACE+ were completed. Two new approaches have been implemented to provide inlets with a more representative turbulent flow.

The first approach generates a random inlet correlated to a specified length scale using an approach similar to that of Klein et al (2003). This method gives the user control of the eddy size at the boundary but does not allow for a range of sizes. Therefore, some development length is still needed to allow the flow to generate the full length of length and time scales. The second method is to simulate the inlet turbulence via an auxiliary solution of the upstream region, utilizing periodic boundary conditions. The resulting periodic outflow boundary condition profile can then be read into the simulation as an inflow boundary condition. This approach provides the full range of length and time scales at the inlet boundary, but only works in cases where a simple channel flow can be defined to characterize the inlet, and is not valid for complex geometries or for inlets with swirl.

### 4.3 SIMVAL Predictions with Improvements

In this quarter, CFDRC reran the 3D LES case of the SIMVAL experiment with $\phi_{inj}$=0.7. Both of the previously discussed improvements were utilized.
Snapshots of temperature contours at various times are shown in Figure 1. It can be seen that the flame anchors on the centerbody, a short distance upstream of the exit. This location of flame

anchoring closely mimics the experiment based on observations of the experimentalists. Previous LES calculations incorrectly predicted the flame being anchored just downstream of the swirler. Another feature seen in Figure 1 is the fine-scale structure of the flame, which is more in-line with what is expected in LES calculations. This is the result of inlet turbulence, which we had not captured in previous LES runs.

Snapshots of $NO_x$ contours at various times are shown in Figure 2. $NO_x$ at the exit is approximately 80 ppm, much higher than extrapolated from the measurements. Unfortunately, the wall heat losses were not correctly input, so the LES calculation had higher bulk temperatures in the combustor and exhaust duct than the experiment. We are currently rerunning the case with the correct heat losses.

This case was very quiet in terms of pressure dynamics. Pressure rms values of ~0.3 psi were predicted. This was in-line with extrapolated pressure rms measurements. Next quarter, we will run LES cases at various $\phi_{inj}$ to see if the code can capture the pressure dynamics measured.

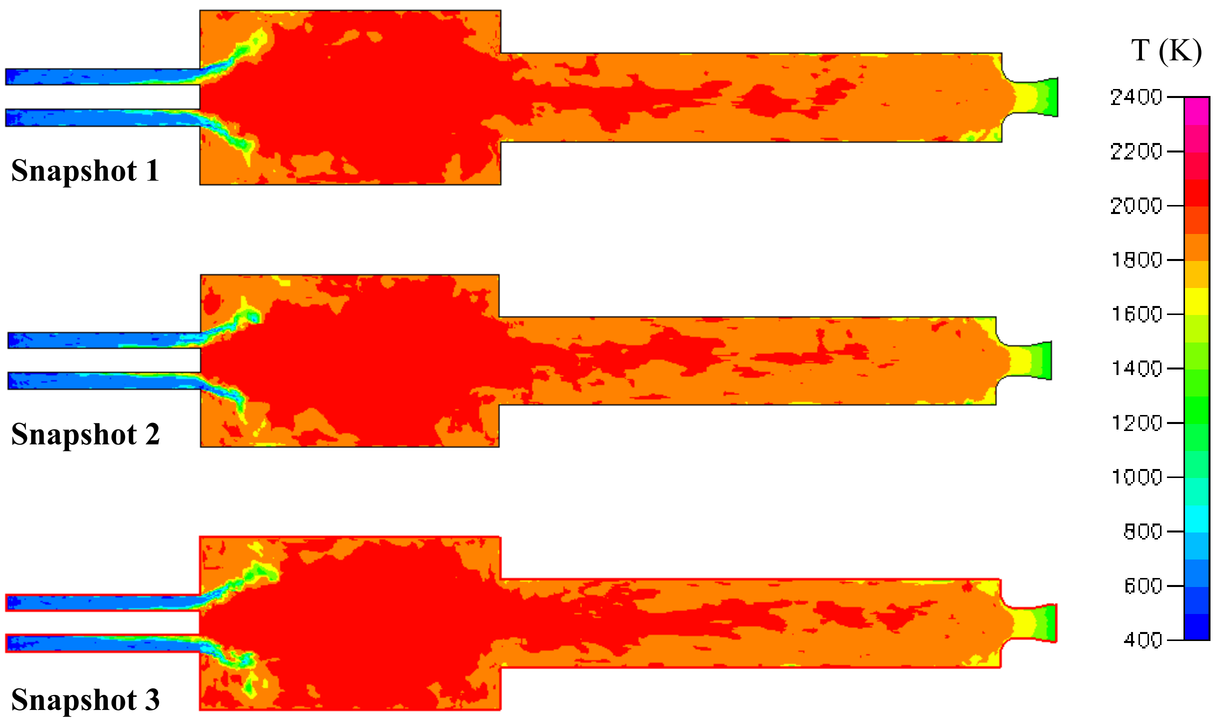


*Figure 1. Snapshots of Temperature Contours*



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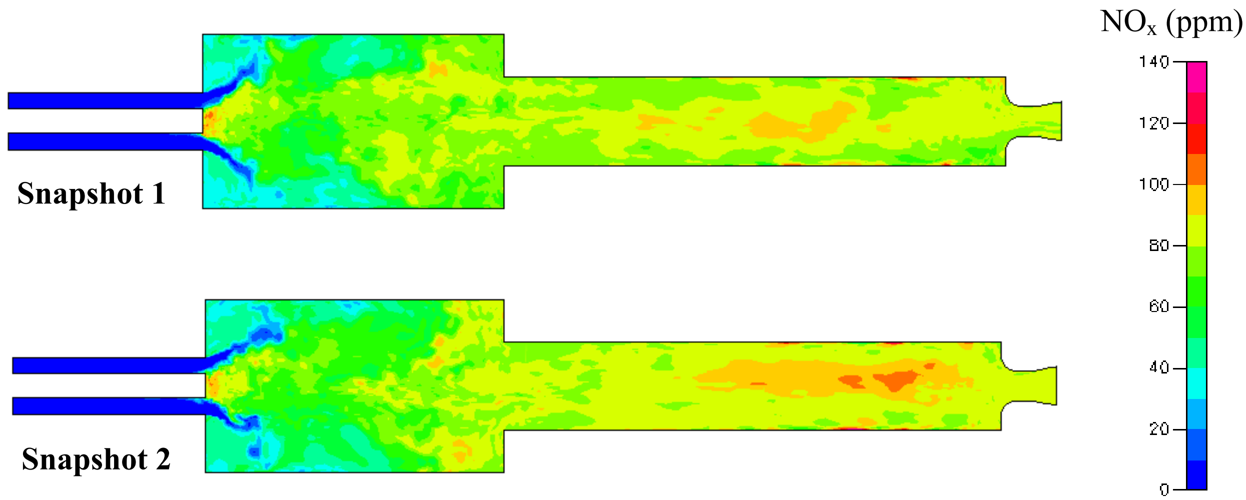
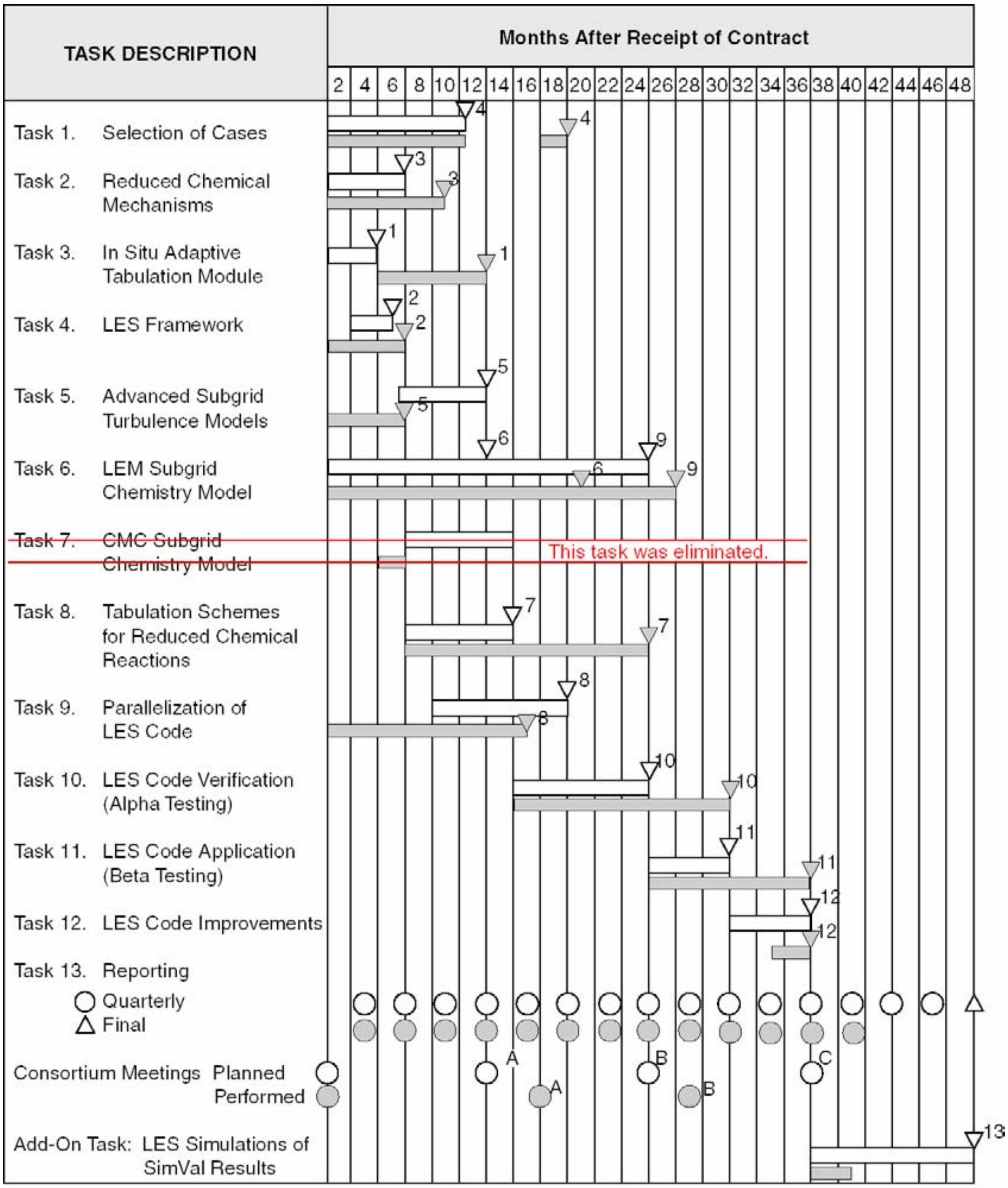



*Figure 2. Snapshots of $NO_x$ Contours*

## 5. REFERENCES

Klein, M., Sadiki, A., Janicka, J., (2003), "A Digital Filter Based Generation of Inflow Data for Spatially Developing Direct Numerical or Large Eddy Simulations," *Journal of Computational Physics*, Vol. 186, pp. 652-665.

## 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 $\phi_{inj}$. 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.