Better Decisions, Better Products
Through Simulation & Innovation

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

Quarterly Technical Progress Report for

April – June 2004

by

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ABSTRACT

Three SIMVAL LES calculations were completed this quarter: ϕ (equivalence ratio) of 1) 0.55, 2) 0.625, and 3) 0.7. The predictions were first analyzed, and then compared to existing experimental data of pressure dynamics, NO_x, and CO emissions. It appears that the combustor flowfield changes for the ϕ of 0.55 case (compared to the other two cases), and this flowfield change results in a slight reduction in the pressure dynamics compared to the ϕ of 0.625 case. The predicted pressure rms values were 1.0 psi or less for the three cases. Good agreement was seen between predicted and measured NO_x emissions for the cases with $\phi = 0.55$ and $\phi = 0.625$. The CO predictions were higher than the measurements, but possible reasons were identified.

A new SIMVAL dataset recorded June, 2004, is being processed and will be transmitted to CFDRC in the near future. The previous two datasets had known deficiencies. This new dataset will be compared to the LES predictions in the next quarter.

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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 fifteenth quarter (April – June 2004) has included further validation of the LES software with SIMVAL experiments. Three equivalence ratio cases (ϕ = 0.55, 0.625, and 0.7) were completed, analyzed, and compared to existing experimental SIMVAL data. Although the SIMVAL data is suspect, still reasonably good agreement of pressure dynamics is seen. NO_x predictions compared well will experimental data for $\phi = 0.55$ and $\phi = 0.625$ (No experimental data were available for $\phi = 0.7$). Predicted CO is much higher than the data, but it is not clear if the predictions or the data are at fault. It appears that the combustor flowfield changes between the ϕ of 0.55 and 0.625 cases, resulting in a slight change in pressure dynamics.

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS

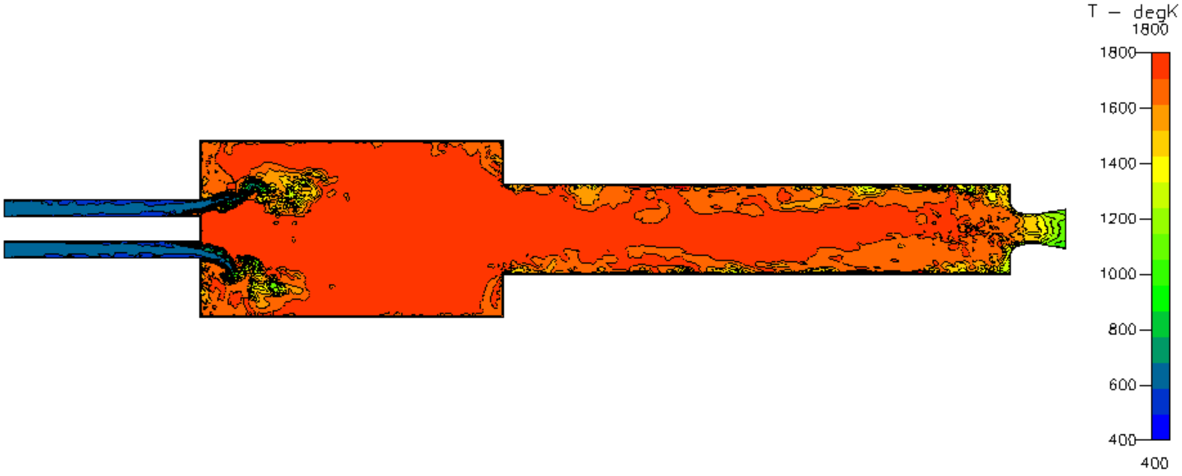
Three LES cases were completed this quarter: 1) ϕ (equivalence ratio) of 0.55, 2) ϕ of 0.625, and 3) ϕ of 0.7. The LES results were studied in some detail, but some questions still remain. The LES predictions were also compared to existing experimental data, realizing the data are suspect, and new data have been recorded (which DOE is processing and will transmit to CFDRC in the near future).

For each case, snapshots of temperature, time-averaged temperature, snapshots of CO emissions, time-averaged CO emissions, snapshots of NO_x, and time-averaged NO_x emissions are presented in Figures 1 through 6, respectively. The temperature snapshots show that fine structures (scales) are being captured, and the unsteadiness that occurs in turbulent flowfields. It is interesting to note that the swirling flow discharging from the premix passage appears to attach to the combustor wall for ϕ's of 0.625 and 0.7, but the swirling flow does not appear to attach to the combustor wall for ϕ of 0.55. This change in the flowfield can change the heat release location, and affect pressure dynamics.

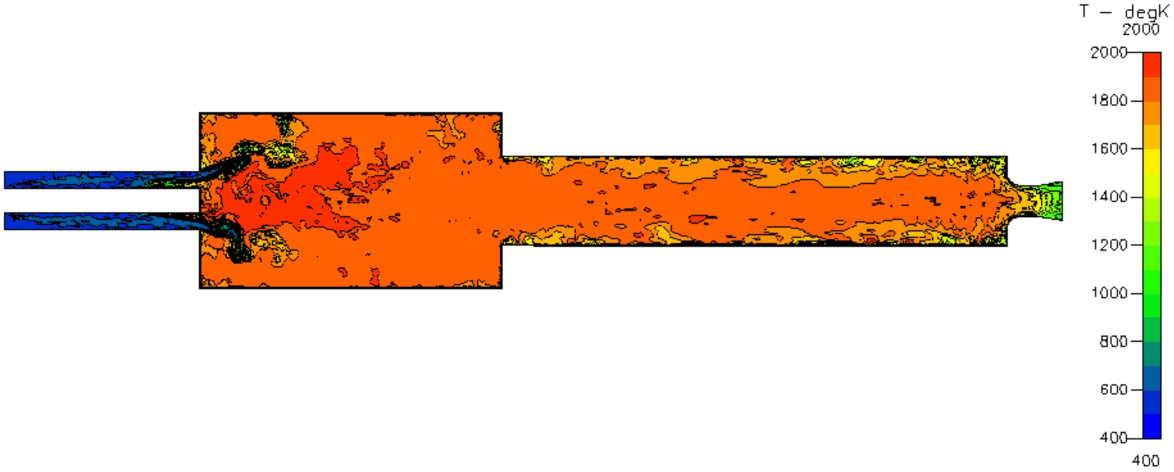
The CO figures (Figure 3 and 4) show that CO is produced near the flamefront, and is oxidized as it travels down the combustor and exhaust duct. In the exhaust duct, the CO levels reduce as the flow travels downstream, due to the temperature dropping (caused by heat loss). Figure 7 shows the measured CO data (at a location approximately eight inches downstream of the choked nozzle) as a function of phi, compared to the LES predictions. The LES predictions are too high. Also shown in Figure 7 is a CO equilibrium curve based on the average temperature just upstream of the choked nozzle. This equilibrium curve exactly matches the data. It is expected that the LES predictions of CO will reach equilibrium (and match the data) if given more time (like the experiment).

The NO_x figures (Figure 5 and 6) show NO_x is created in the combustor, and continues to form in the exhaust duct, especially for the ϕ of 0.7 case. It is important to accurately resolve the heat loss in the exhaust duct for accurate SIMVAL NO_x predictions, especially for ϕ of 0.7. Figure 8 shows a comparison of predicted and measured NO_x emissions. Good agreement is seen for the cases with ϕ of 0.55 and 0.625. For ϕ of 0.7, the NO_x prediction seems to be much greater than the extrapolated measurements. However, it is known that NO_x increases exponentially with flame temperature, so the ϕ of 0.7 predictions may not be as far off as it seems in Figure 8.

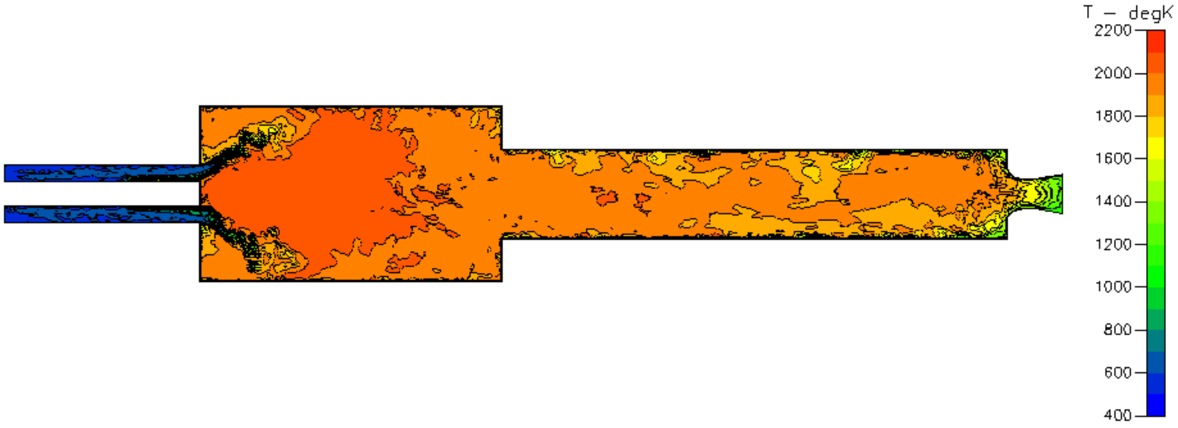
Figure 9 presents the LES predictions of pressure dynamics at the three equivalence ratios, compared to existing experimental data. The predicted pressure rms values in the combustor are 0.4 psi, 1.0 psi, and 0.7 psi for ϕ's of 0.7, 0.625, and 0.4, respectively. It can be seen that the first set of experimental data recorded a change in the dynamics at phi of 0.6, while the second set of experimental data did not. Both of these sets of data are suspect, based on leakage and other test problems. Per emails from DOE, it seems the third set of experimental data has "low" pressure dynamics (CFDRC has not yet seen the data). Comparisons will be made once we receive the data.



(a) $\phi = 0.\ 55$

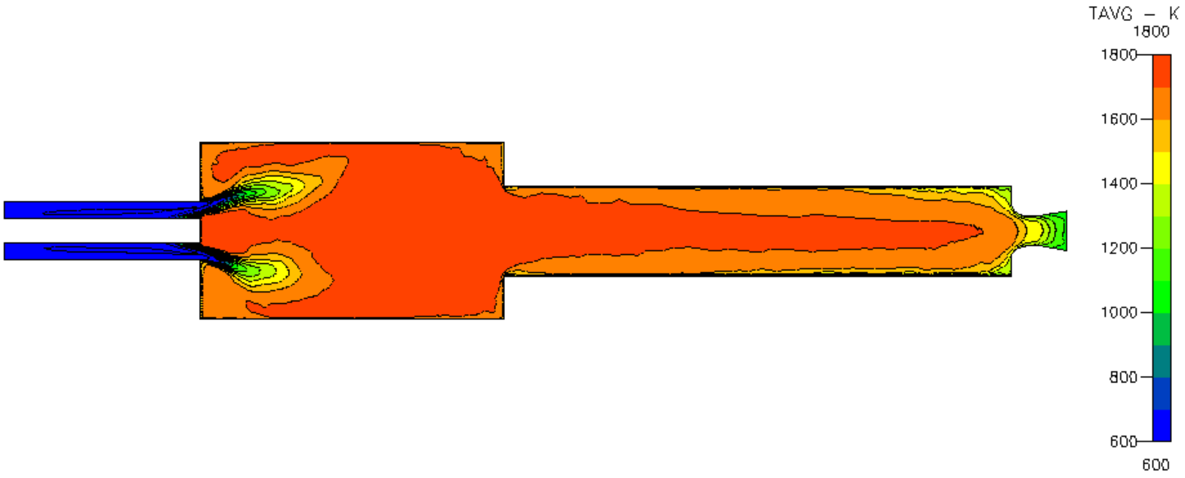


(b) $\phi = 0.\ 625$

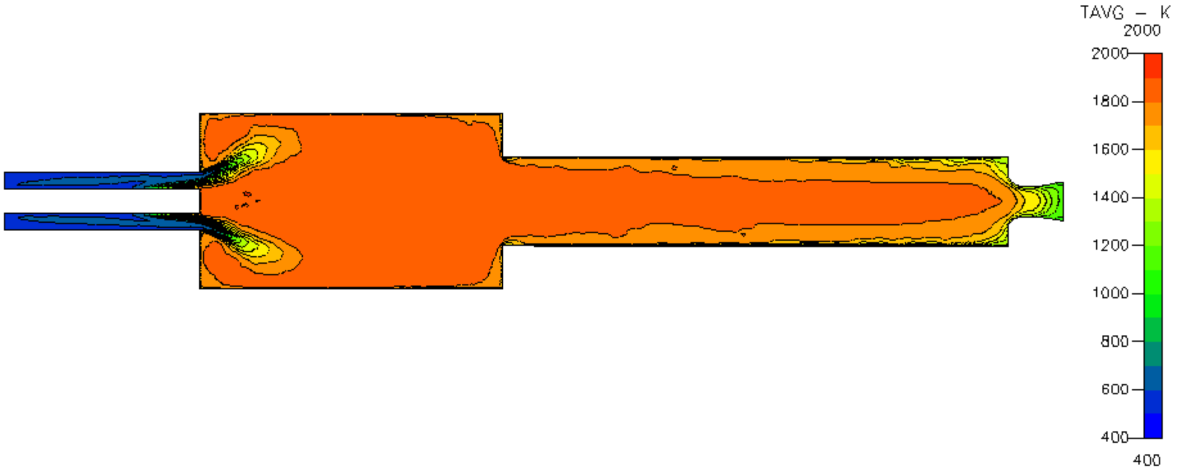


(c) $\phi = 0.7$

Figure 1. Snapshots of Temperature (Note Different Scales)



(a) $\phi = 0.\ 55$



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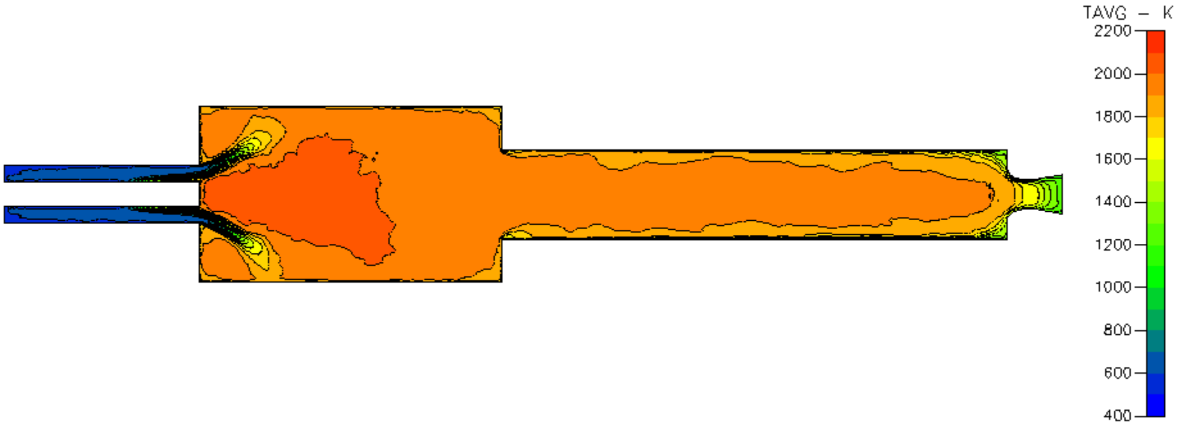
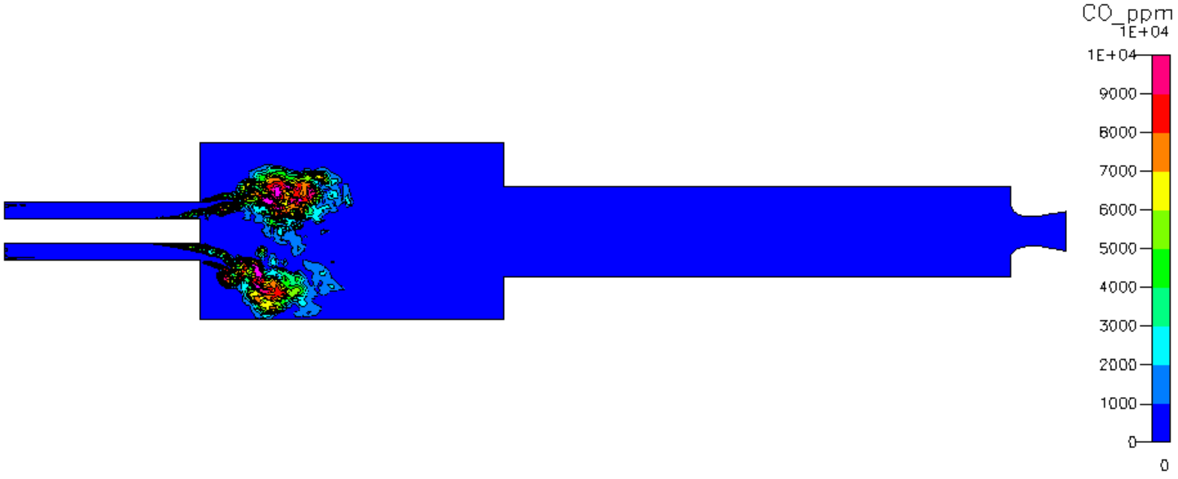
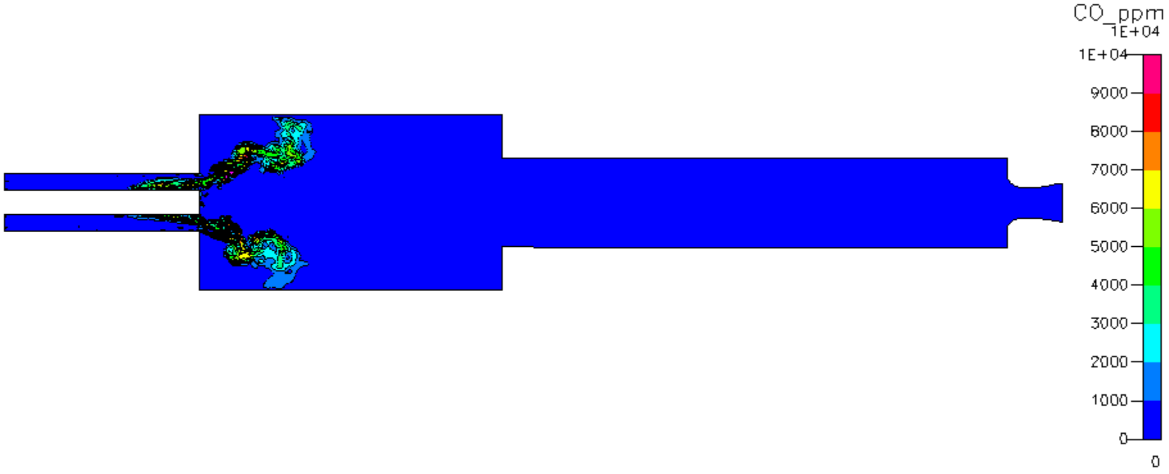


(c) $\phi = 0.7$

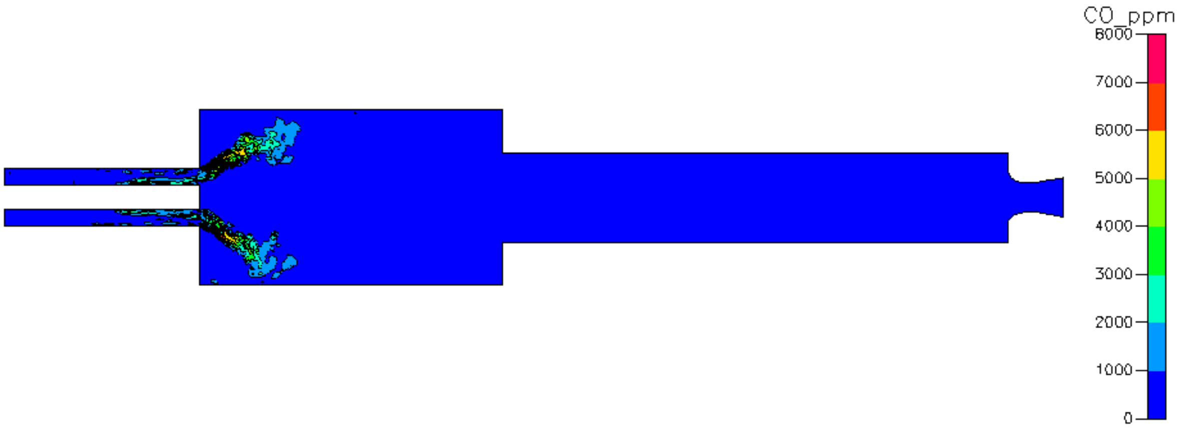
Figure 2. Time-averaged Temperature Contours (Note Different Scales)



(a) ϕ = 0. 55

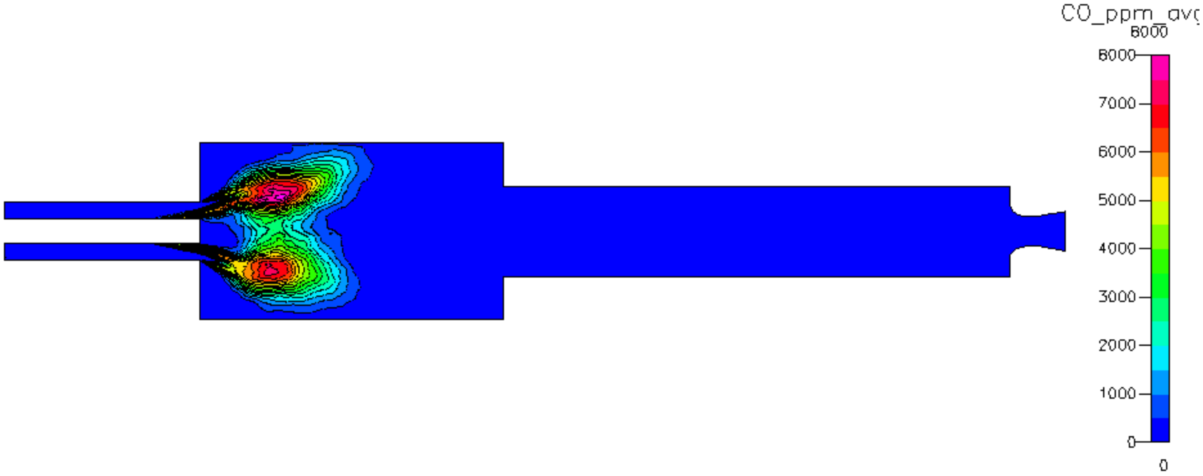


(b) ϕ = 0. 625

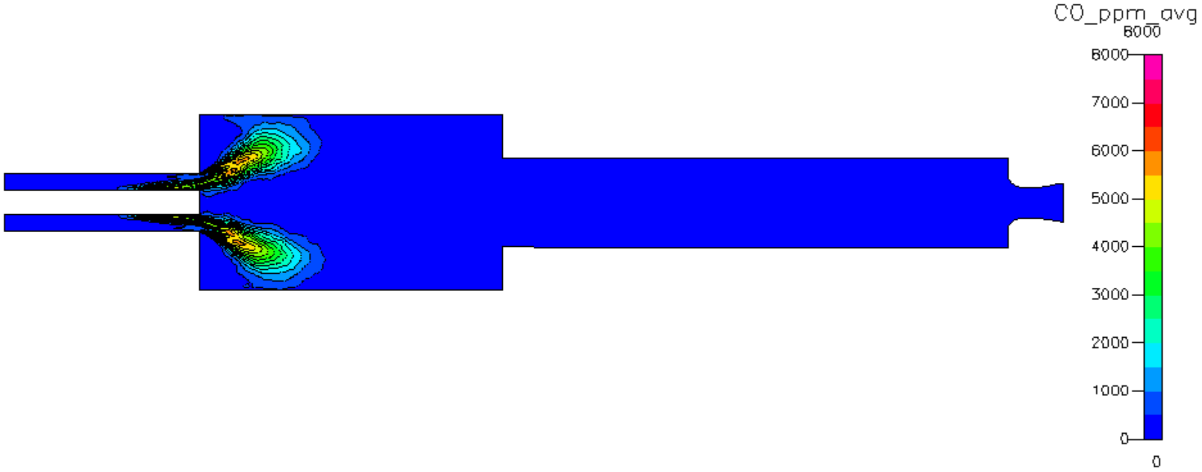


(c) ϕ = 0.7

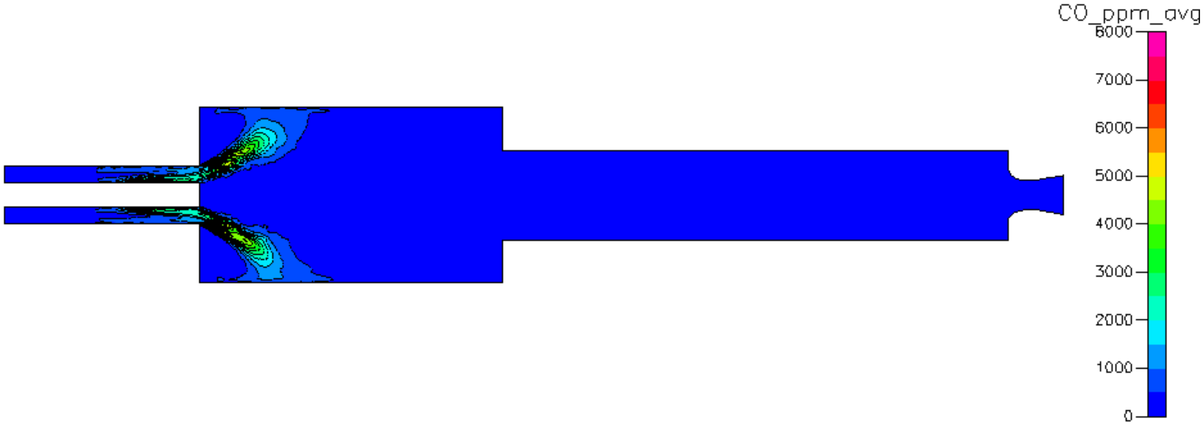
Figure 3. Snapshots of CO Emissions



(a) ϕ = 0. 55

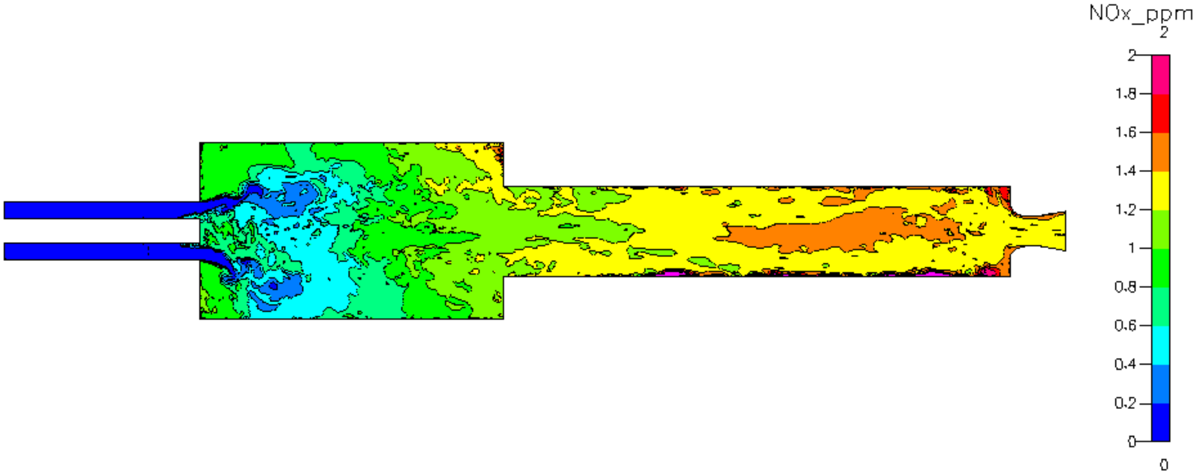


(b) ϕ = 0. 625

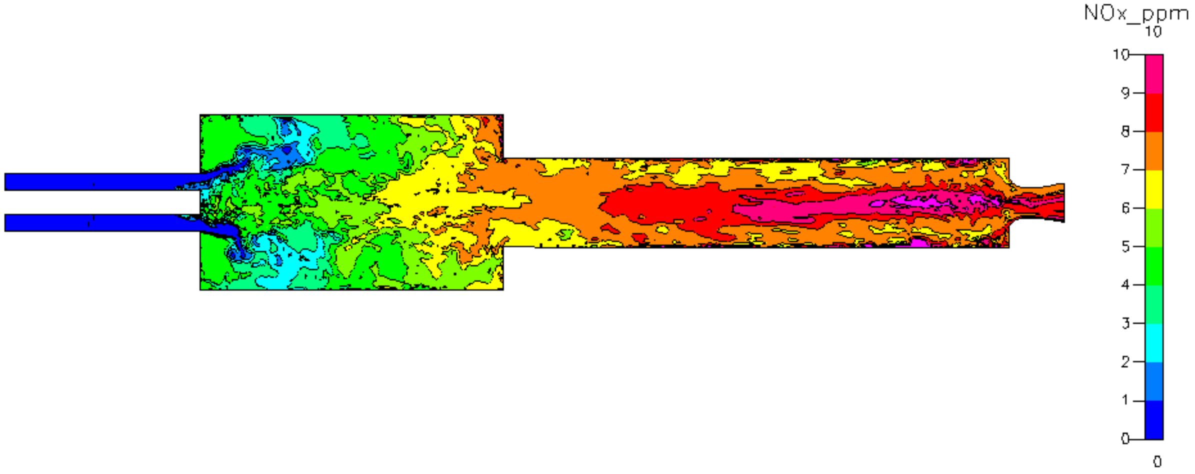


(c) ϕ = 0.7

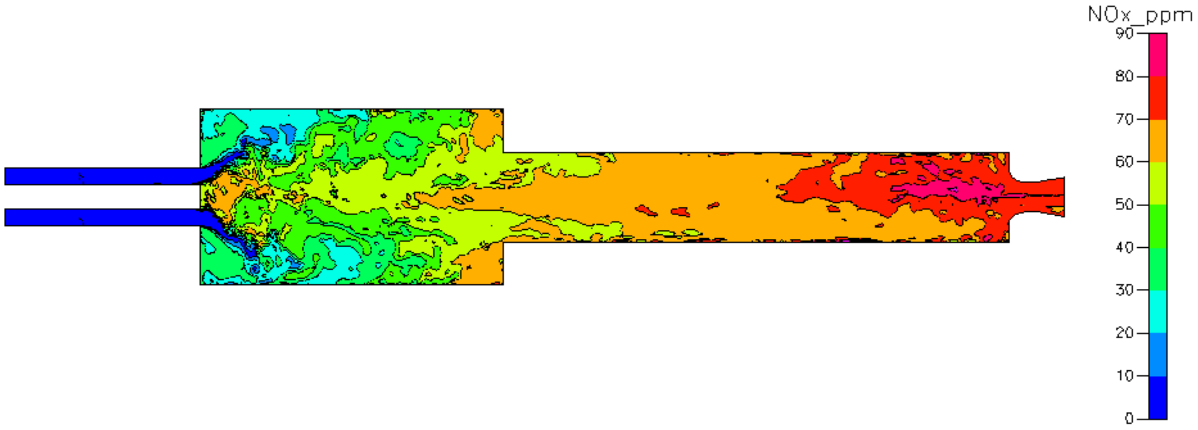
Figure 4. Time-averages CO Emissions



(a) $\phi = 0.55$

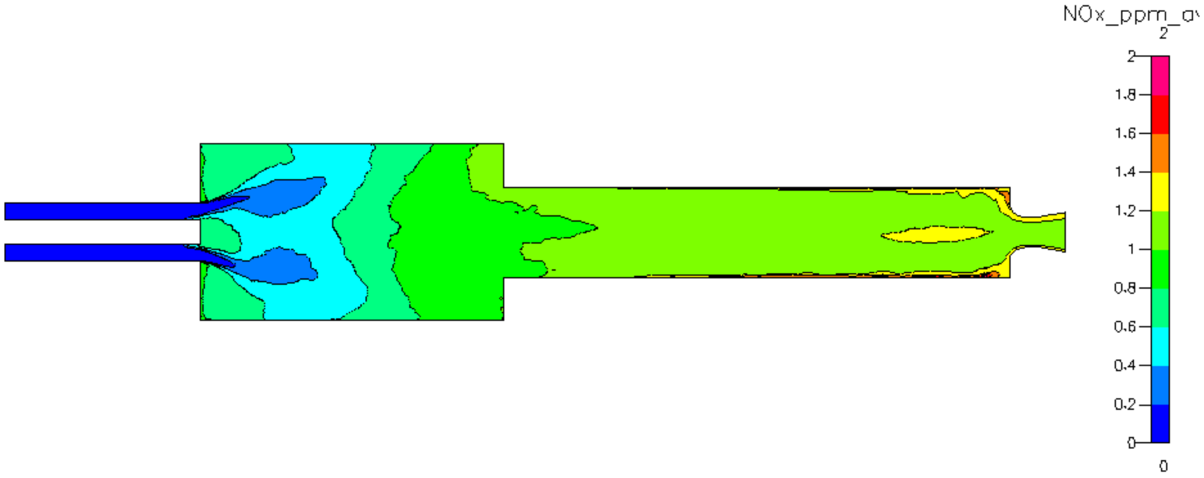


(b) $\phi = 0.625$

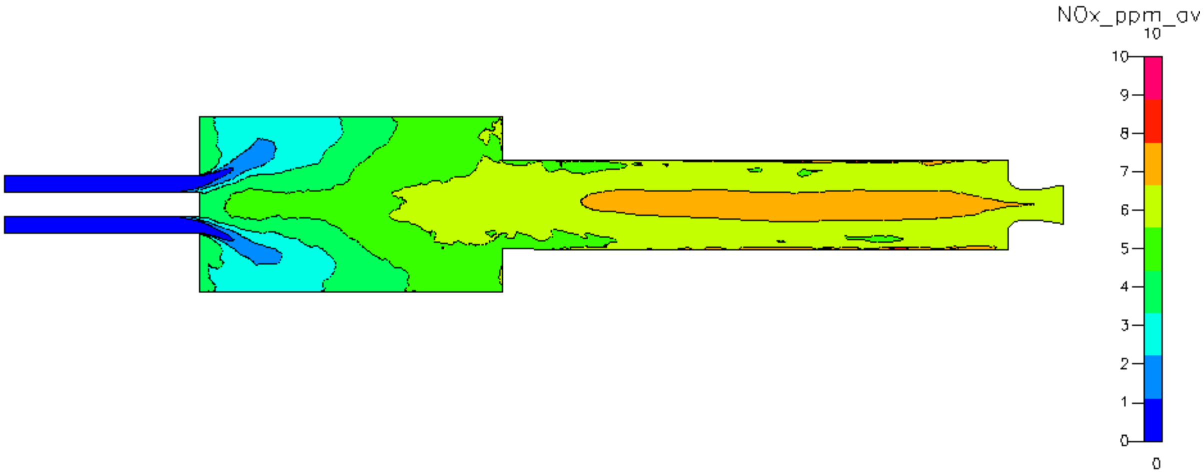


(c) $\phi = 0.7$

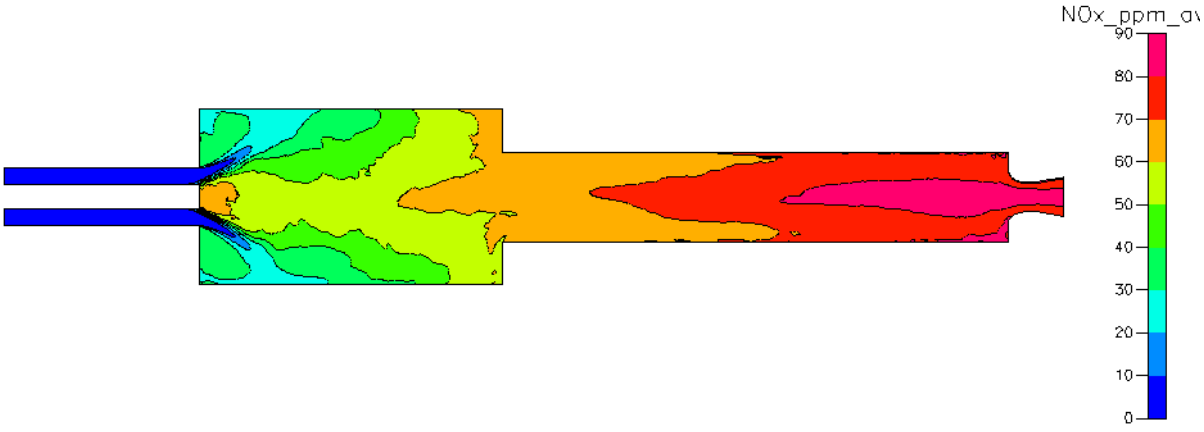
Figure 5. Snapshots of NO_x *Emissions (Note Different Scales)*



(a) $\phi = 0.55$



(b) $\phi = 0.625$



(c) $\phi = 0.7$

Figure 6. Time-averaged NO_x Contours (Note Different Scales)

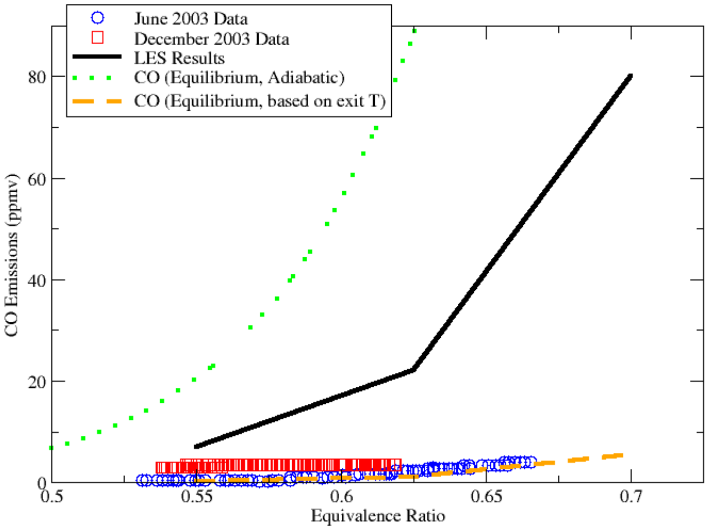


Figure 7. CO Emissions Pressure Plot

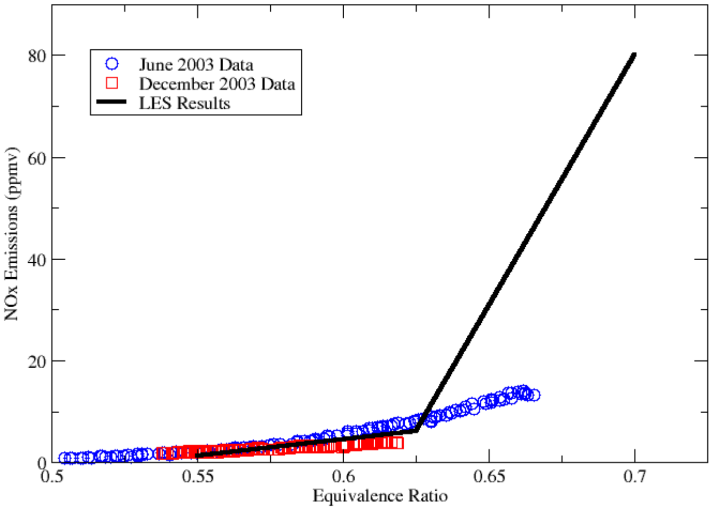


Figure 8. NO_x Emissions Pressure Plot

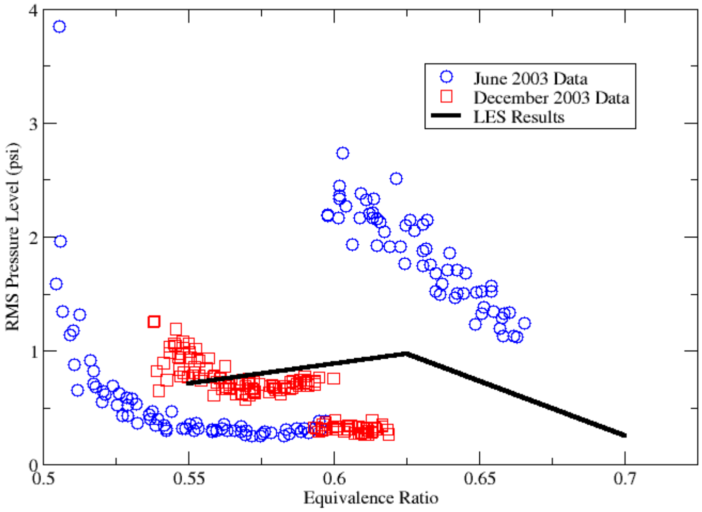
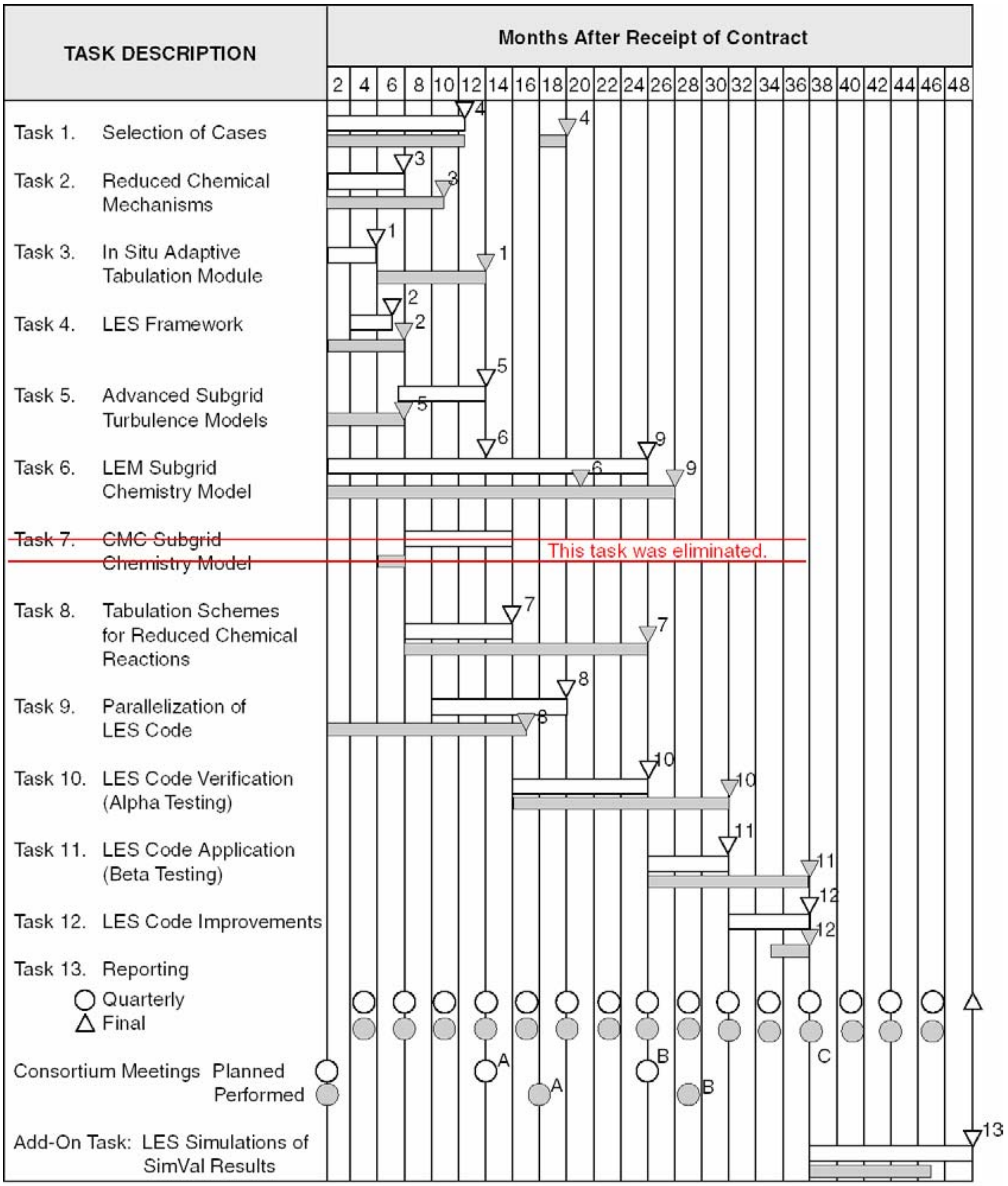


Figure 9. RMS Pressure Level Plot

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 LES predictions will be compared to experimental data recorded June, 2004. Any discrepancy will be studied, and recommendations for future work discussed. The final report will be written and submitted to DOE. The final LES code will be available to consortium members, and to the public-at-large.