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

Quarterly Technical Progress Report for

April - June 2003

by

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ABSTRACT

Application and testing of the new combustion Large Eddy Simulation (LES) code for the design of advanced gaseous combustion systems is described in this 11th quarterly report. CFD Research Corporation (CFDRC) has developed the LES module within the parallel, unstructured solver included in the commercial CFD-ACE+ software. In this quarter, validation and testing of the combustion LES code was performed for the DOE-Simval combustor. A very limited amount of data was available from DOE. Also, beta testing by six consortium members was performed for various burner and combustor configurations.

In the quarter remaining, CFDRC will continue to work closely with the beta testers to complete their tasks. The beta testers will compare their predictions with experimental measurements and other numerical calculations. Unfortunately, the beta testers are running behind schedule due to computer platform issues, longer that expected training time, and other unexpected delays. Only one beta tester (Virginia Tech) has completed reacting flow cases at the present time. To ensure that meaningful, reacting flow cases are run by the beta testers, we have extended the date of beta testing completion to mid-August, and have invested more manpower to help the beta testers.

At the end of this project (October 1, 2003), a final released version of the software will be available for licensing to the general public.

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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) were utilized to help develop and implement these advanced submodels into the unstructured, parallel CFD flow solver. 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. During the last year, six industrial and academic partners are using the combustion LES code and exercising it on problems of their choice. Final feedback and optimizations will then be implemented in the final release version of the combustion LES software that will be licensed to the general public.

2. EXECUTIVE SUMMARY

Work in this eleventh quarter (April - June 2003) has included further validation of the LES software. Predictions have been performed for the DOE-SimVal lean premixed combustor. Beta testing by gas turbine and industrial burner companies continued, but more effort is needed to complete their effort.

Next quarter, completion of the following tasks are planned:

1. Complete beta testing of the code.
2. Implement LES software improvements based on beta testers' feedback.
3. Submit final report to DOE

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS

4.1 DOE-SIMVAL Combustor Validation

Calculations of the DOE SimVal lean premixed combustor were performed at CFDRC. The SimVal combustor will provide experimental data that can be used to validate combustion CFD codes, with particular emphasis on understanding combustion instability and variable fuel effects at actual gas turbine combustor conditions. Initial experimental data has been taken and released by Dan Maloney at DOE-NETL. CFDRC participated in a panel session at the June 2003 IGTI Gas Turbine Expo in Atlanta. Bob Malecki, of Pratt & Whitney, presented the simulation results and the comparisons to experimental data. The experimental data was not available to CFDRC or the other participants. The results from this panel session and subsequent post-dictive calculations will be discussed here.

The baseline geometry of the SimVal combustor includes well-defined acoustic boundaries with a choke plate immediately upstream of the swirl vanes and a choked nozzle at the downstream end of a resonant section. Figure 1 shows the baseline geometry. The baseline operating conditions included:

Air Mass Flow-Rate	0.26 kg/sec
Inlet Air Temperature	600 K (620 F)
Equivalence Ratio	0.47 - 0.7
Pressure	~ 4.5 atm (varied with equivalence ratio)

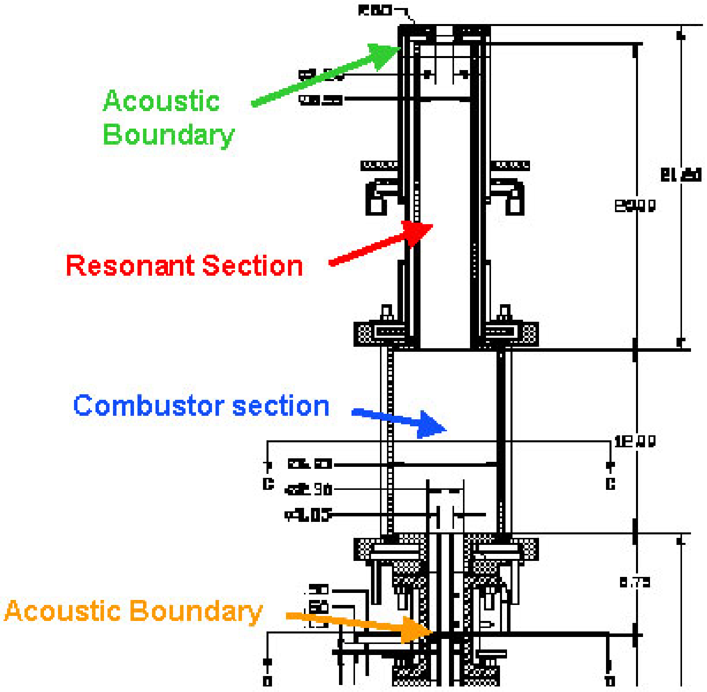


Figure 1. Baseline Geometry for SimVal Combustor

Initial 3D non-reacting calculations of the slot swirler were performed by Bob Malecki of Pratt & Whitney. These full-swirler calculations provided the inlet profiles for the reacting CFD model used by CFDRC. The predicted axial and tangential velocity profiles, as well as the swirl angle in the annular injector region, are shown in Figure 2. It is clear that a recirculation bubble forms just downstream of the swirl vanes. At 2 inches upstream of the combustor dump, the flow is all positive and the swirl angle varies from 55 to 65 degrees. The profiles at the 2 inch location were used in the CFDRC reacting flow models and were applied 7.75 inches upstream of the combustor dump, where the choke plate and swirl vanes are located.

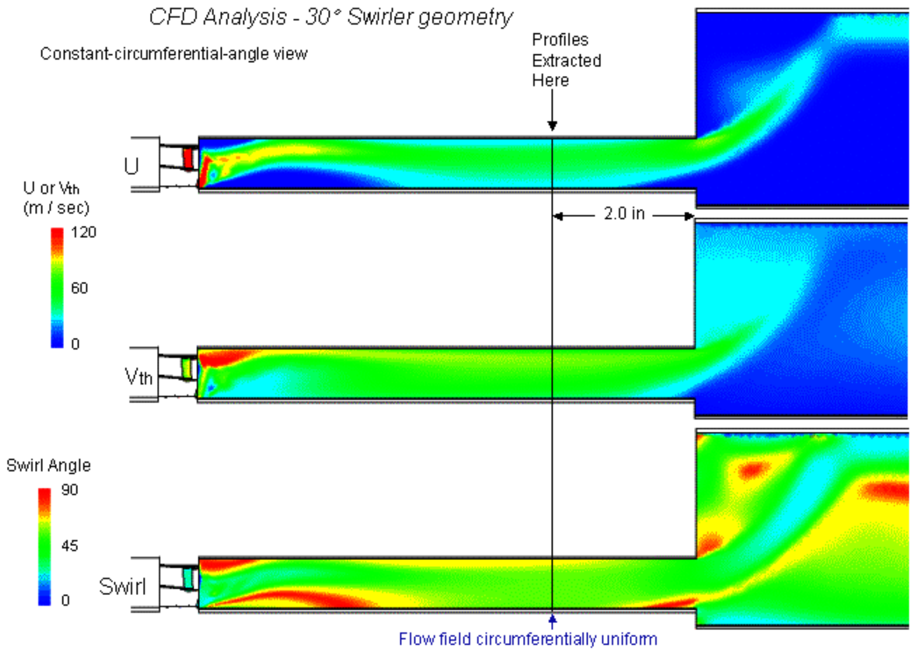


Figure 2. P&W Predicted Non-Reacting Flowfield Through Swirler and Injector Annular Passage

A fixed mass flow with completely premixed reactants was assumed at the inlet with the appropriate profiles on velocity, pressure, and temperature from the P&W simulation. The fully burned conditions provided a choked flow at the exit nozzle throat. An extrapolated boundary condition was used at the supersonic nozzle exit. The 2D axisymmetric geometry used ~15,000 cells and the 3D geometry required ~1,500,000 cells.

Both RANS, unsteady RANS, and LES calculations were performed. Second-order accurate spatial and temporal differencing methods were utilized. The 2-step reaction model assumed finite-rate methane oxidation to CO and then finite-rate CO oxidation to equilibrium products. De-coupled NO_x chemistry that included thermal, nitrous, and prompt mechanisms was included. The 2-dimensional (mixture fraction and reaction progress) assumed PDF method was used to account for turbulence and chemistry interactions. Since the flow was perfectly premixed, mean (or filtered) reaction rates were only affected by fluctuations in the reaction progress. The transport equation for the variance of the reaction progress depends on the turbulent mixing due to subgrid scales for LES. The Ck coefficient for this turbulent mixing term was changed from a value of 2 (for RANS) to a value of 200 for LES. This was needed to produce realistic results.

If the standard value of 2 were used, then unrealistically high variances would occur near the burning flame zone and these high variances would in turn reduce the mean reaction rate significantly so that some unburnt fuel would escape the combustor exit. This Ck coefficient could be computed locally using LES filtering techniques and will be implemented in CFD-ACE+.

It was found that wall temperatures in the model were an important boundary condition, since heat loss had a large effect on the emissions in this long residence time (~30 msec) combustor. Initially, hot 1650 K walls were assumed in the air-cooled, quartz lined combustor. Cold 658 K walls were assumed in the dome and water-cooled resonant section. Predicted temperatures for equivalence ratios of 0.5, 0.6, and 0.7 are shown in Figure 3. The reduction in combustor temperature with downstream distance is apparent due to the heat loss. A difference of 250 K between adiabatic equilibrium and the mean exit temperature was observed. It is interesting to observe the hot product gases in the injector along the ID for the ϕ=0.7 case. The upstream propagation of flame into the injector was quite sensitive to boundary conditions and models.

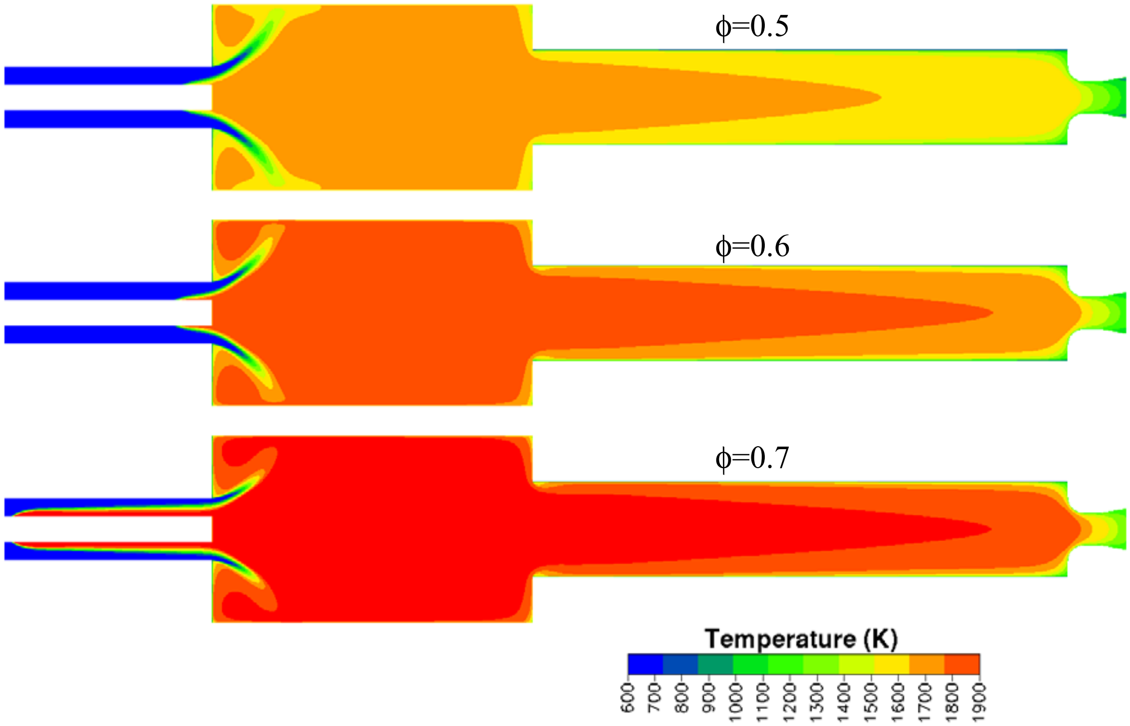


Figure 3. Predicted RANS Temperatures (RNG k-ε) for ϕ = 0.5, 06, and 0.7

If for example, the calculations were performed with the more viscous standard k-e model, rather than the RNG k-e model, then the flame would not penetrate very far up into the injector. Figure 4 shows temperature predictions using the standard k-e model. The experimental evidence seemed to indicate that the flame went upstream only about 0.5-1 inches, not the 6 or 7 inches seen in the RNG k-ε results.

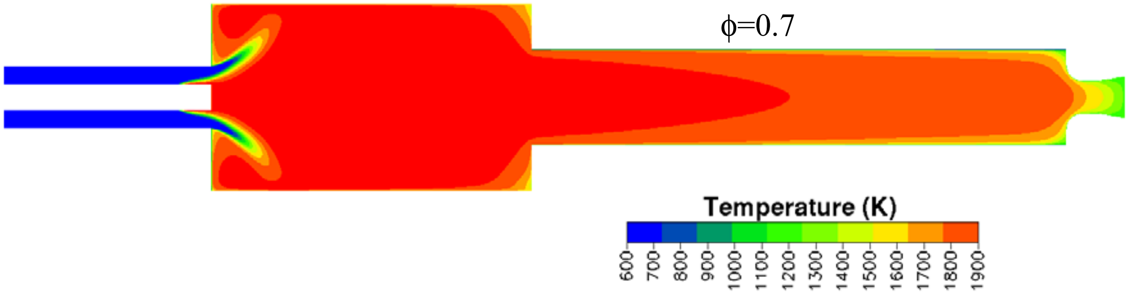


Figure 4. Predicted Steady-state Temperature for Standard k-ε model (ϕ=0.7)

LES calculations were performed for 2D axisymmetric and full 3D geometries. The LES timesteps were 5E-6 seconds and statistics were accumulated over several flow-through times. The sensitivity of the turbulence model was also apparent in LES for predicting the flame propagation (flashback) up inside the injector. Figure 5 shows predicted mean temperatures using different subgrid turbulence models; Localized Dynamic Turbulent Kinetic Energy (LDKM) and Smagorinsky. The LDKM results clearly show the flame propagation up inside the barrel. The use of a finer grid in the injector, with y+ values of ~2, also produced this upstream flame propagation. The more viscous Smagorinsky model did not allow the flame to propagate upstream into the injector. The higher viscosities seem to allow more heat loss at the walls. In addition, the higher viscosities could make the flow have less tendency to separate along the injector ID and/or reduce local flame reaction rates. It is not clear that the wall boundary conditions are being treated correctly for the LDKM model. The consistent treatment of velocities and subgrid kinetic energy at the walls will be studied in more detail.

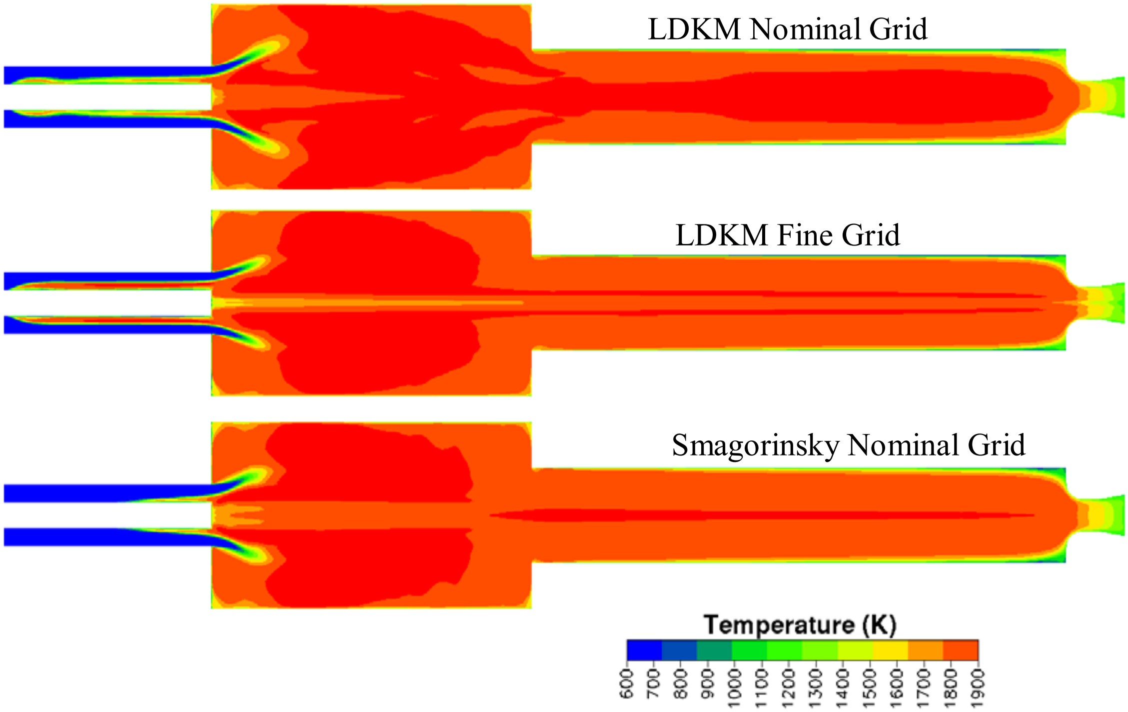
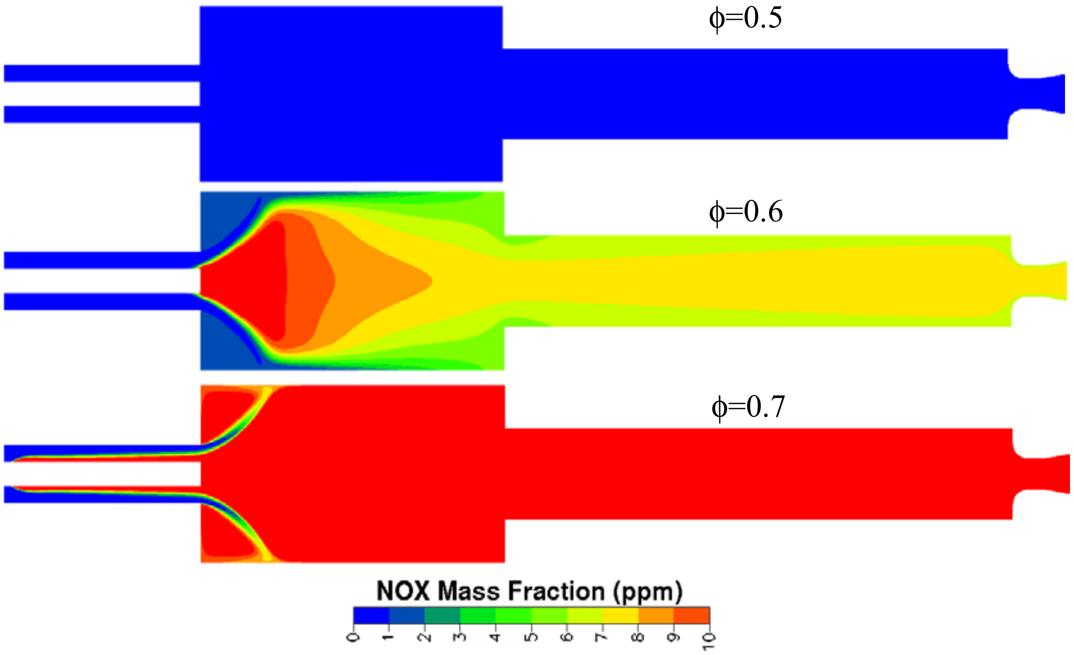


Figure 5. Predicted Temperatures Using LES with Subgrid Turbulence Models of LDKM and Smagorinsky (ϕ=0.65) and With Nominal and Fine Grids (15,000 vs. 30,000 cells)

The NO_x and CO emissions just downstream of the exit nozzle were measured and were compared to the model predictions. Figure 6 shows the predicted NO_x emissions within the flowfield and the area-averaged exit value. Most of the NO_x is formed in the combustor central recirculation zone. The NO_x mixes out in the downstream section of the combustor and remains relatively constant in the resonant section. A ϕ=0.65 case was also simulated since the data only went up to a ϕ of 0.67. A good comparison with data is obtained at the leanest conditions. The model overpredicts the NO_x at ϕ=0.6 and above. This overprediction could be due to the assumed heat loss in the CFD model. To understand the sensitivity of heat loss on the NO_x predictions, the ϕ=0.65 case was run with the cooler combustor wall temperatures that were measured (~1350 K vs. 1650 K). The cooler wall temperatures reduced the NO_x predictions by 30%, giving fairly good agreement with the data (see Figure 7).

The LES cases were run with 1650K wall temperatures. The use of LES with the LDKM model did not substantially change NO_x emissions compared to RANS at ϕ = 0.65 (see Table 1). The Smagorinsky LES results produced lower NO_x than LDKM (see Table 1). This was primarily due to the higher heat loss and reduced flame area for the Smagorinsky case compared to the LDKM case. Figure 8 shows 3D LES results of NO_x rate and vorticity. It can be seen that the NO_x rate increases slightly in regions of high vorticity in the reacting shear layer. The NO_x rate decreases near the combustor walls where significant heat loss occurs. At the time of this report, the 3D LES calculations had not run long enough to get NO_x statistics.



	Exit NO_x (ppm) Pred.	Meas.
ϕ=0.5	1	1
ϕ=0.6	7	6
ϕ=0.7	62	N/A

Figure 6. Predictions and Measurements of NO_x Emissions at ϕ=0.5, 0.6, and 0.7 (1650 K Wall Temperatures)

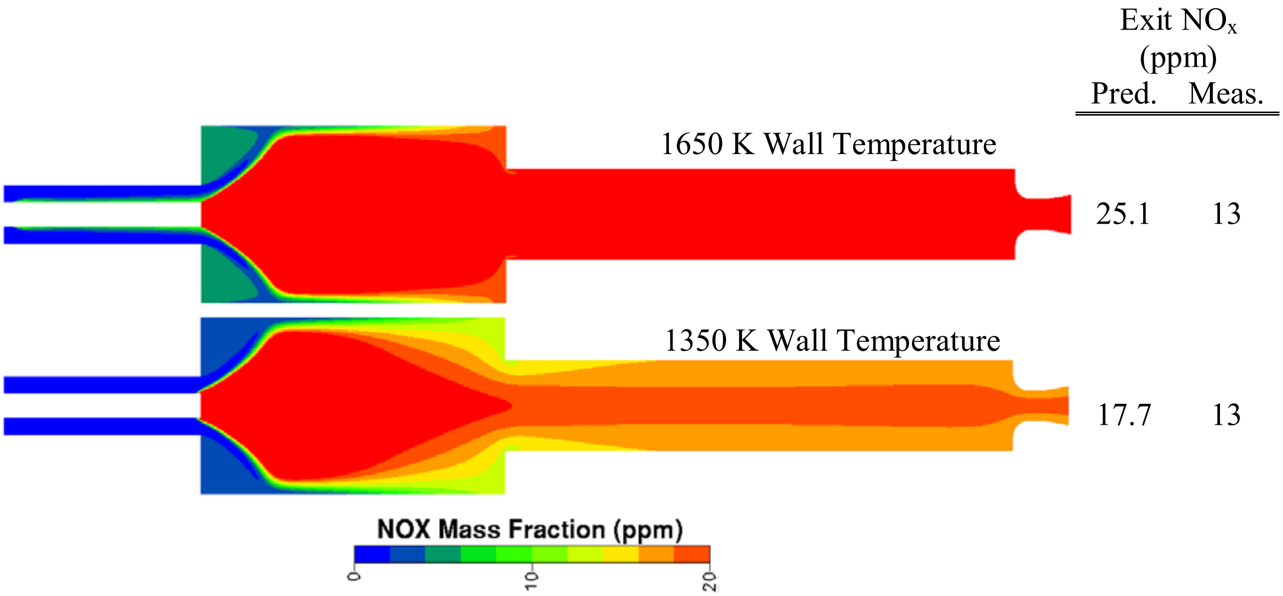
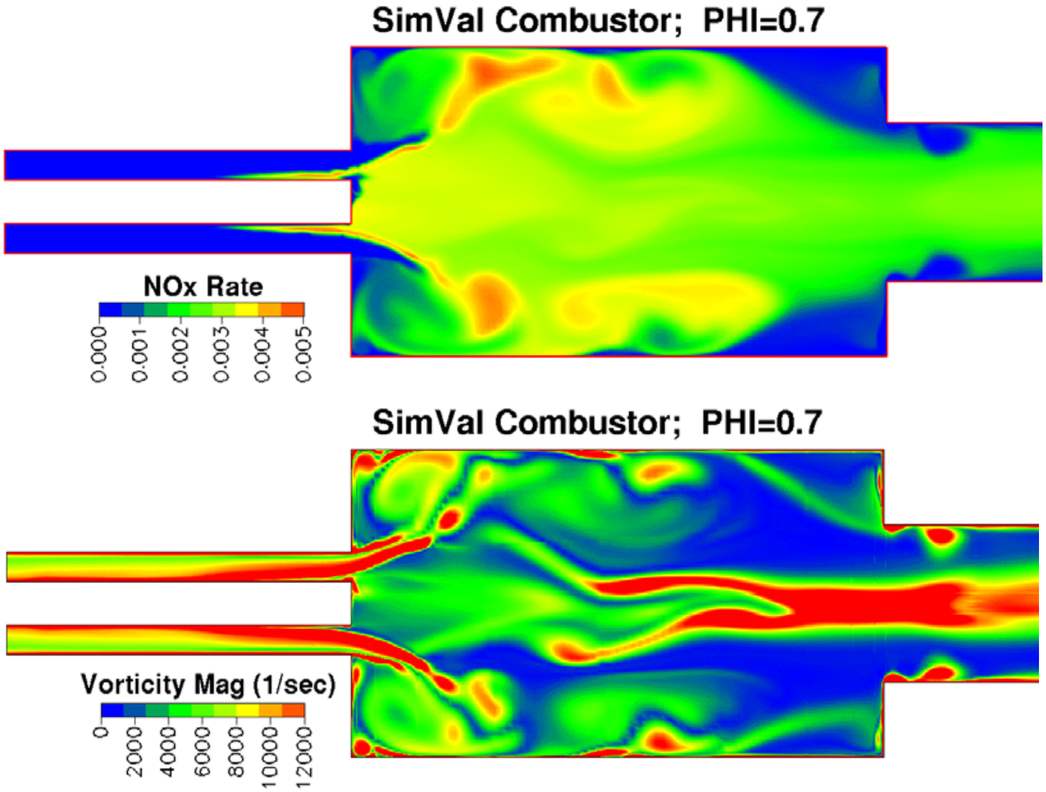


Figure 7. Predictions and Measurements of NO$_x$ Emissions at ϕ=0.65 (1650 vs. 1350 K Combustor Wall Temperatures)

Table 1. Summary of Cases Run

Case #	**ϕ**	**GEOM**	**TWALL**	**Wall Grid**	**TURB**	**RANS**	**LES (rms)**	**NO$_x$ (ppm)**	**NO$_X$ Data (ppm)**	**CO (ppm)**	**CO Data (ppm)**	**Flash back**
1	0.5	2D	1650K	$y^+ > 20$	RNG	√		1	1	2.5	0	N
2	0.6	2D	1650K	$y^+ > 20$	RNG	√		7	6	12	2	N
3	0.7	2D	1650K	$y^+ > 20$	RNG	√		62	~25	41	~10	Y
4	0.65	2D	1650K	$y^+ > 20$	RNG	√		25	13	22	4	N
5	0.65	2D	1350K	$y^+ > 20$	RNG	√		18	13	17	4	N
6	0.7	2D	1650K	$y^+ > 20$	k-ε	√		52	~25	30	~10	N
7	0.65	2D	1650K	$y^+ > 20$	LDKM		(0.2)*	25	13	58	4	Y
8	0.65	2D	1650K	$y^+ \sim 2$	LDKM		(0.9)*	?	13	?	4	Y
9	0.65	2D	1650K	$y^+ > 20$	Smag		(1.2)*	18	13	40	4	N
10	0.7	3D	1650K	$y^+ > 20$	LDKM		(0.4)*	?	~25	?	~10	Y
11	0.6	2D	1650K	$y^+ > 20$	LDKM		?	10	6	30	2	Y

*Dominant frequencies 1200 – 1400 Hertz, function of temperature.

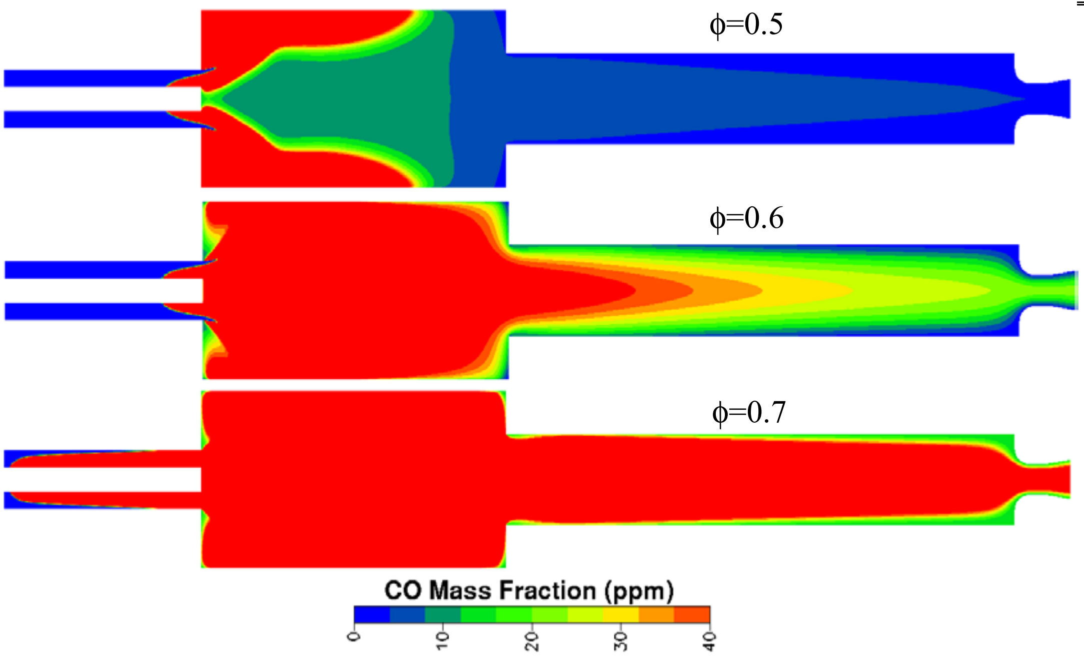


SimVal Combustor; PHI=0.7

SimVal Combustor; PHI=0.7

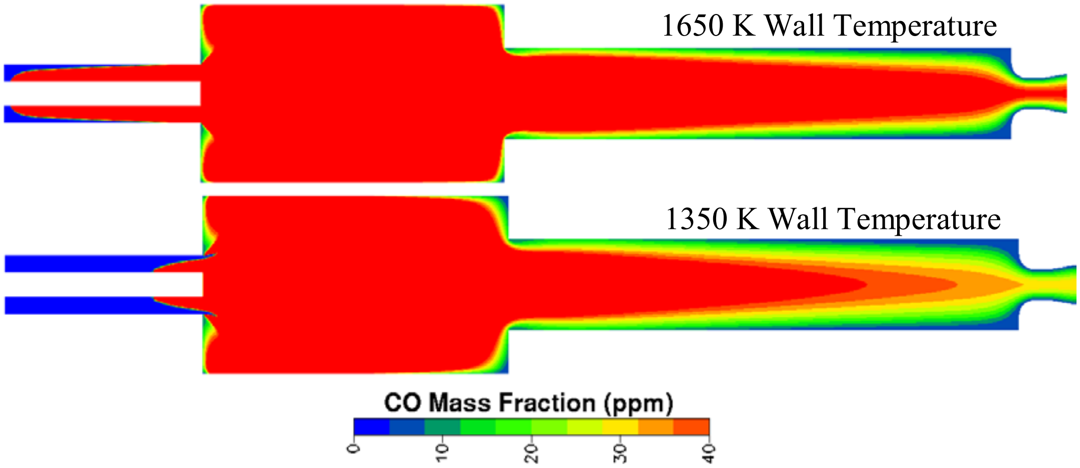
Figure 8. 3D LES Snapshot of Filtered NO_x *Source Term and Vorticity Magnitude (*ϕ*=0.7, LDKM)*

CO emissions were also computed and compared to experimental data. These results are shown for RANS in Figure 9. The predicted CO emissions at the combustor exit were very close to equilibrium. The predictions of CO are consistently higher than the measurements. The underpredicted heat loss is one likely reason for the discrepancy. Cases at a ϕ of 0.65 were run with lower combustor wall temperatures and the CO was reduced by 25%, providing better agreement with the data (see Figure 10), but still substantially more than the measurement. It is unclear at the present time whether the measurements are in error, or the predictions are in error.



Exit NO_x (ppm)	
Pred.	Meas.
2.5	0
12	2
41	N/A

Figure 9. RANS Predictions of CO Emissions (ϕ=0.5, 0.6, and 0.7)



Exit CO (ppm)	
Pred.	Meas.
22.2	4
16.5	4

Figure 10. RANS Predictions of CO Emissions (ϕ=0.65 and Twall = 1350 K and 1650 K)

A comparison of measured and predicted dynamic combustor wall pressure was also performed. Figure 11 shows the tabulated results with rms pressure as a function of equivalence ratio. It can be seen that the measured unsteady pressure becomes very large as lean blowout is reached. Also, as the equivalence ratio is varied from 0.59 to 0.61, the combustor becomes very unstable, until finally reaching lower levels of unsteadiness at equivalence ratios higher than 0.67.

The predictions were relatively stable using the LDKM LES model at equivalence ratios of 0.5, 0.6, and 0.7. The 2D LES model did not predict the lean blowout correctly. At ϕ's of 0.6 and 0.7, it is difficult to determine if the model is doing an adequate job or not. Thus, an additional case of ϕ=0.65 was run. Here again, the choice of turbulence model for the LES had an impact on the instability as would be expected. The Smagorinsky model gave the best result, as it predicted rms pressure levels around 1.2 psi. The LDKM produced low levels around 0.2 psi. The LDKM was re-run with a finer grid and rms levels of 0.9 psi were detected. The unsteady RANS results did not produce any measurable level of instability. It is likely that the unsteady RANS is not capable of picking up the high frequencies that are excited in this non-fuel-time-lag system. The excited frequencies were between 1200 and 1400 Hz, depending on combustor temperature. These frequencies correspond to the longitudinal mode of the combustor, and were similar to those frequencies that were measured. Further calculations need to be performed around ϕ=0.6 to determine what is causing the sudden increase and then decrease in combustion instability. It may be that the flame zone shifts closer to the dome as the equivalence ratio is increased to ϕ=0.6, giving high instability levels. Then the flame becomes more distributed along the ID of the injector as the ϕ is further increased above 0.6. This distributed flame in the injector would suppress the coupling of unsteady heat release and acoustics.

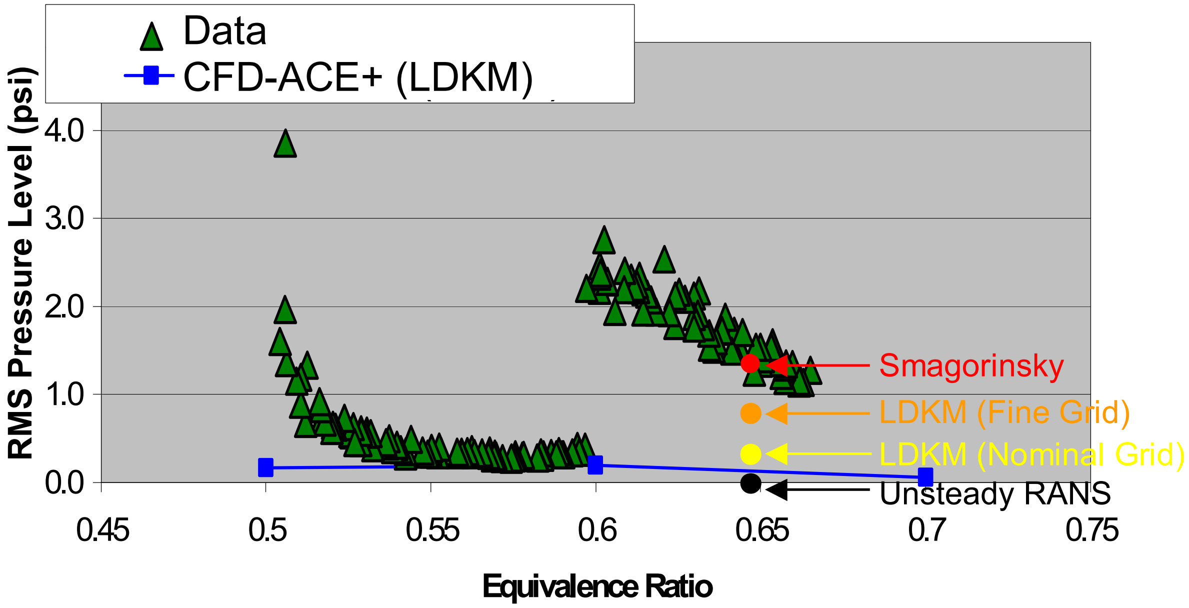


Figure 11. Comparison of Measured and Predicted (2D LES) RMS Pressure Levels in SimVal Combustor

4.2 Beta Test Results

Solar Turbines: Solar Turbines is running a case that simulates fuel-air mixing in an industrial gas turbine premixer. The premixer geometry includes an upstream plenum that feeds a swirler with downstream fuel spokes. The premixer annular passage then dumps into a combustor geometry. A 60 degree sector was modeled that included 1 swirl vane and two fuel spokes. Cyclic boundary conditions were needed for this configuration.

Solar desired to use a grid from Grid-Pro, another commercial grid generator. A substantial amount of time was spent by CFDRC to modify CFD-ACE+ so that Grid-Pro grids could be run (see previous quarterly report). In the end, we had to generate the grid with CFD-GEOM (CFDRC's grid generation package), and export the grid to Solar. Solar is now running CFD-ACE+ with this grid.

Rolls Royce: Rolls Royce is using the CFD-ACE+ software at the Pittsburgh Supercomputer site. The are setting up a case for modeling the Sydney Swirl Burner. Results should be available by mid-August, 2003.

Babcock & Wilcox (B&W): Alan Sayre at Babcock and Wilcox (B&W) is running a simulation of the Sandia/BERL furnace. The 300 kW swirl-stabilized natural gas burner was designed and built by the International Flame Research Foundation (IFRF). The burner is circumferentially symmetric with a bluff center body containing 24 radial natural gas injection holes. For details, see the last quarterly progress report. Combustion air is supplied by a blower and introduced through the annular air zone and swirled using IFRF swirl blocks. The burner has the capability for flue gas recirculation (FGR) and fuel staging, but was operated only in the single-stage mode without FGR for the baseline validation case.

B&W has an 8 PC Linux cluster for running the software. The computational grid of the BERL furnace was generated using CFD-GEOM. Cyclic boundaries were used and the case was run in parallel on the 8 Pcs. Figure 12 shows the computational grid. Currently, B&W is having difficulty converging the solution of each timestep, and we are looking closely at their setup. One aspect that seems to hinder convergence is the gridding near the centerline. They plan on running reacting cases once the cold flow LES solution is obtained.

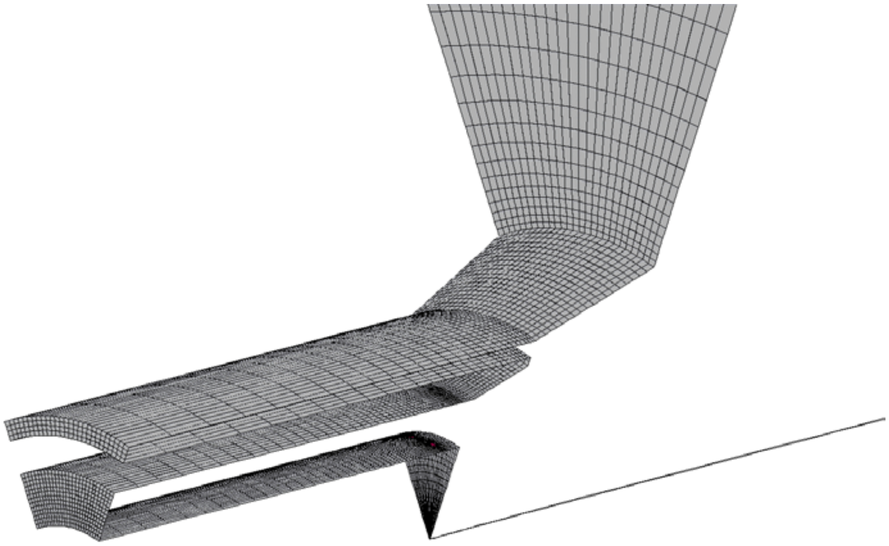


Figure 12. Computational Grid of the Burner Region for the B&W LES Furnace Simulation

Virginia Tech: Virginia Tech has set up and run 2D axisymmetric LES calculations of their swirl stabilized combustor using the CFD-ACE+ code. The combustor includes a lean premixed swirl injector with a round head bluffbody and a diverging conical section (quarl). The quarl is followed by a step that forms the combustor dump. Figure 13 shows a combustor schematic with central and outer recirculation zones that stabilize the flame. We expect to receive their final report in early August, 2003.

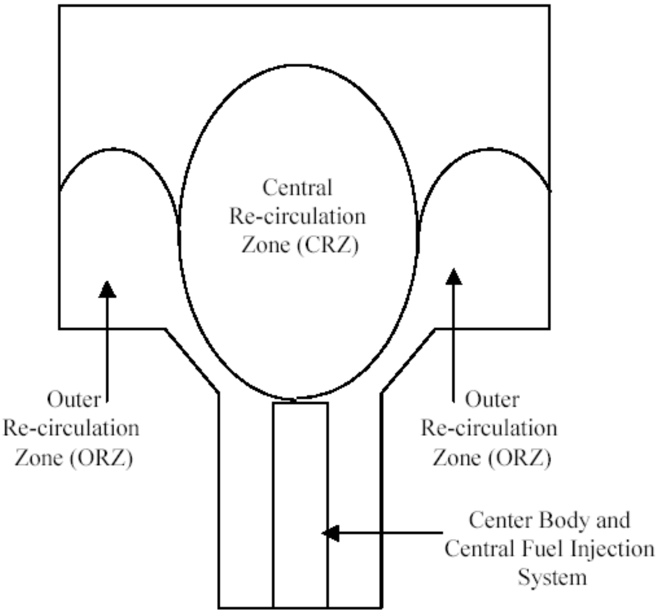


Figure 13. Schematic Showing Recirculation Zones in the Virginia Tech Swirl Stabilized Combustor

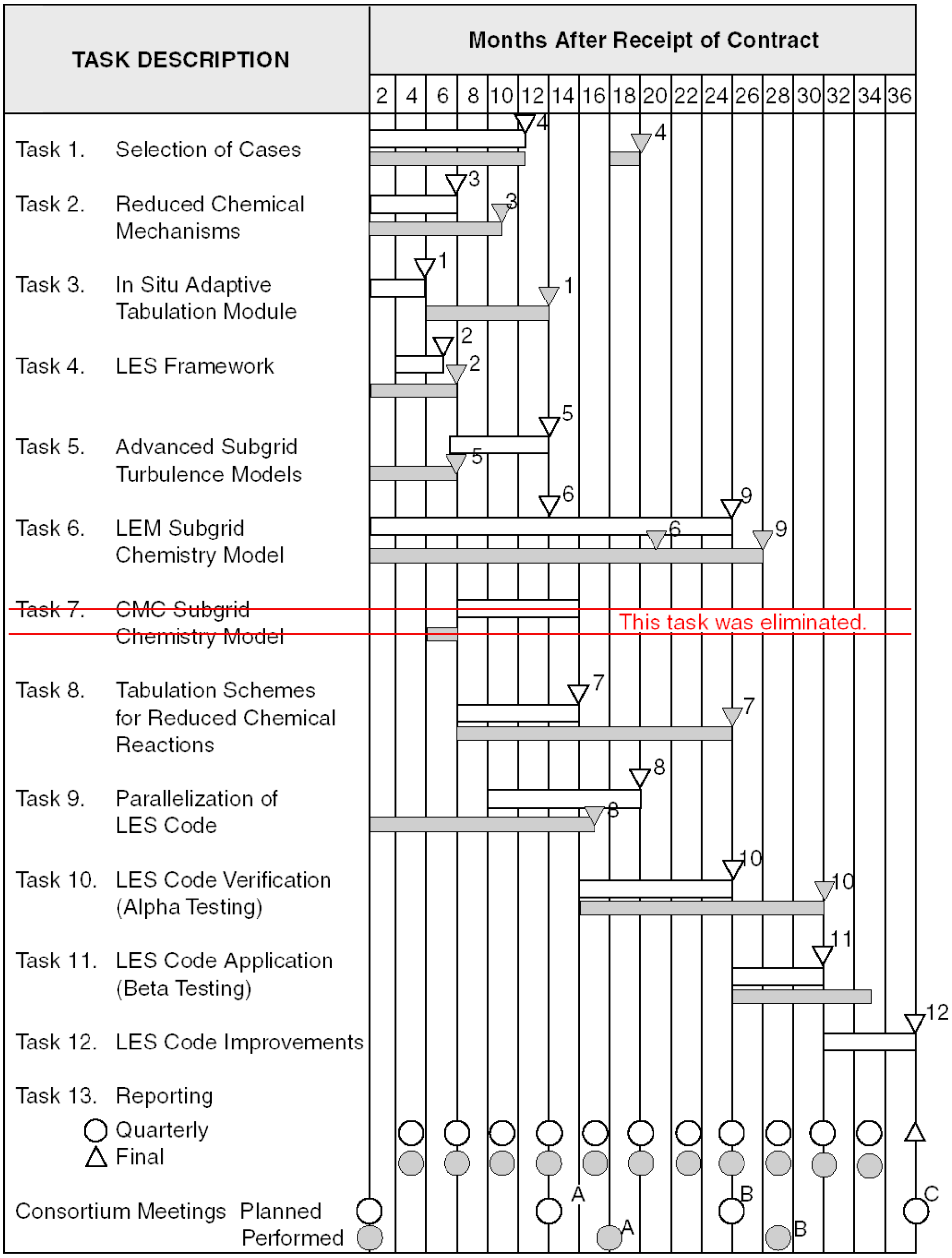
Coen: Paul Matys at Coen has set up a cluster of 16 Linux Pcs and has installed the CFD-ACE+ software. Coen is running a bluff-body stabilized flame for evaluating the LES software. LES predictions with the new CFD-ACE+ software will be compared with Fluent and with experimental data. We expect Coen to finish the analysis and submit a report to CFDRC by mid-August, 2003.

University of California, Irvine (UCI): UCI completed one RANS case and one LES case of cold flow past a conical bluffbody. They experienced a multitude of installation challenges (not related to CFD-ACE+ issues) that greatly restricted their time to run meaningful cases. They also could not run cases longer than 24 hours on their cluster. Thus, their reported analyses are only considered preliminary, and are not included in this quarterly report.

5. REFERENCES

Fornaciari, N., Schefer, R., Paul, P., Sanford, R., Claytor, L., and Lubeck, C., 1994, "Users Guide to the Burner Engineering Research Laboratory," Presented to the American Flame Research Committee/Japanese Research Committee at the Pacific Rim International Conference on Environmental Control of Combustion Processes, October 16-20, Maui, Hawaii.

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

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

During the next quarter, the following work is planned:

1. Support beta testers.
2. Itemize code improvements recommended by beta testers.
3. Write final report