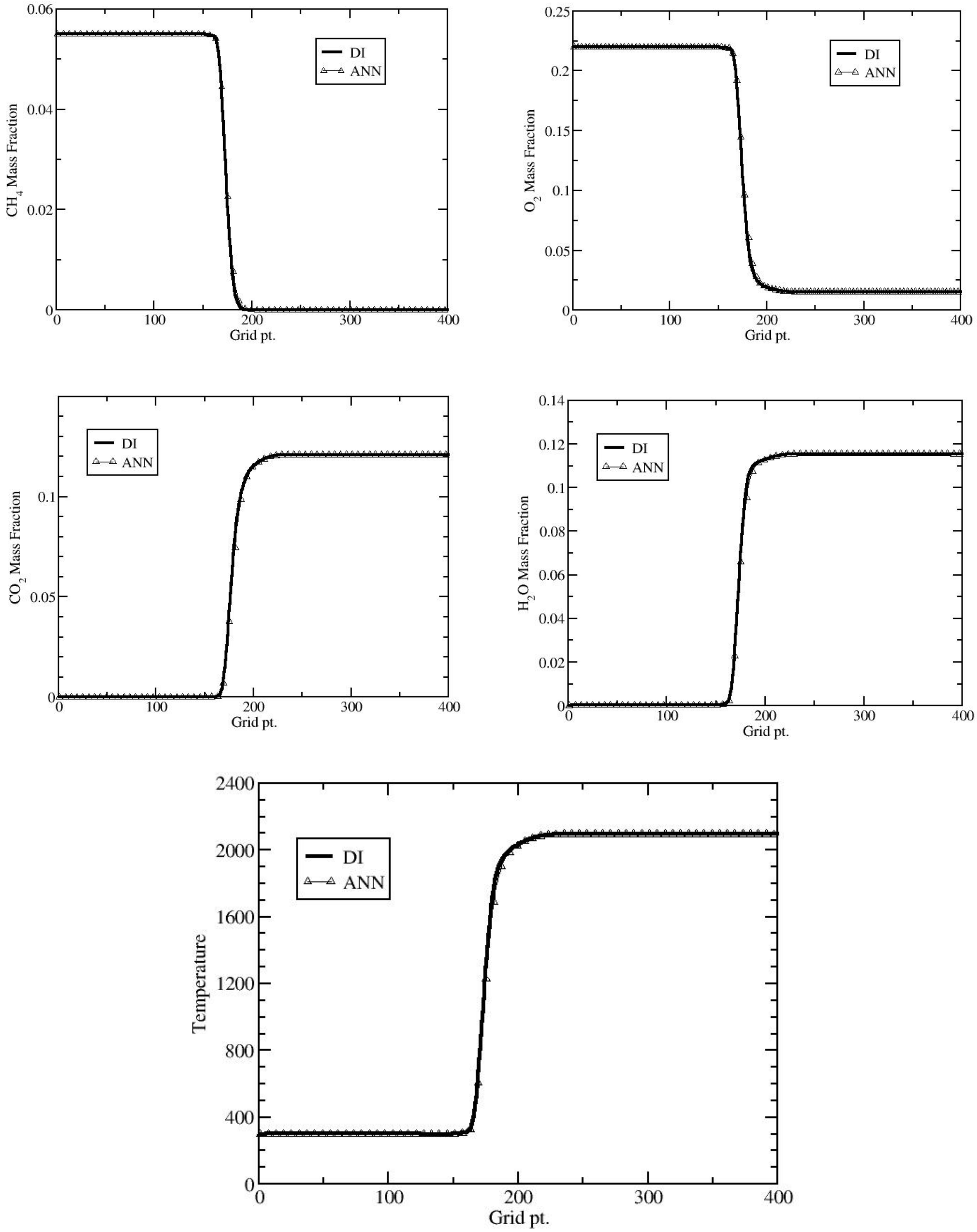


Figure 8. 2D DNS Comparison: DI vs. ANN

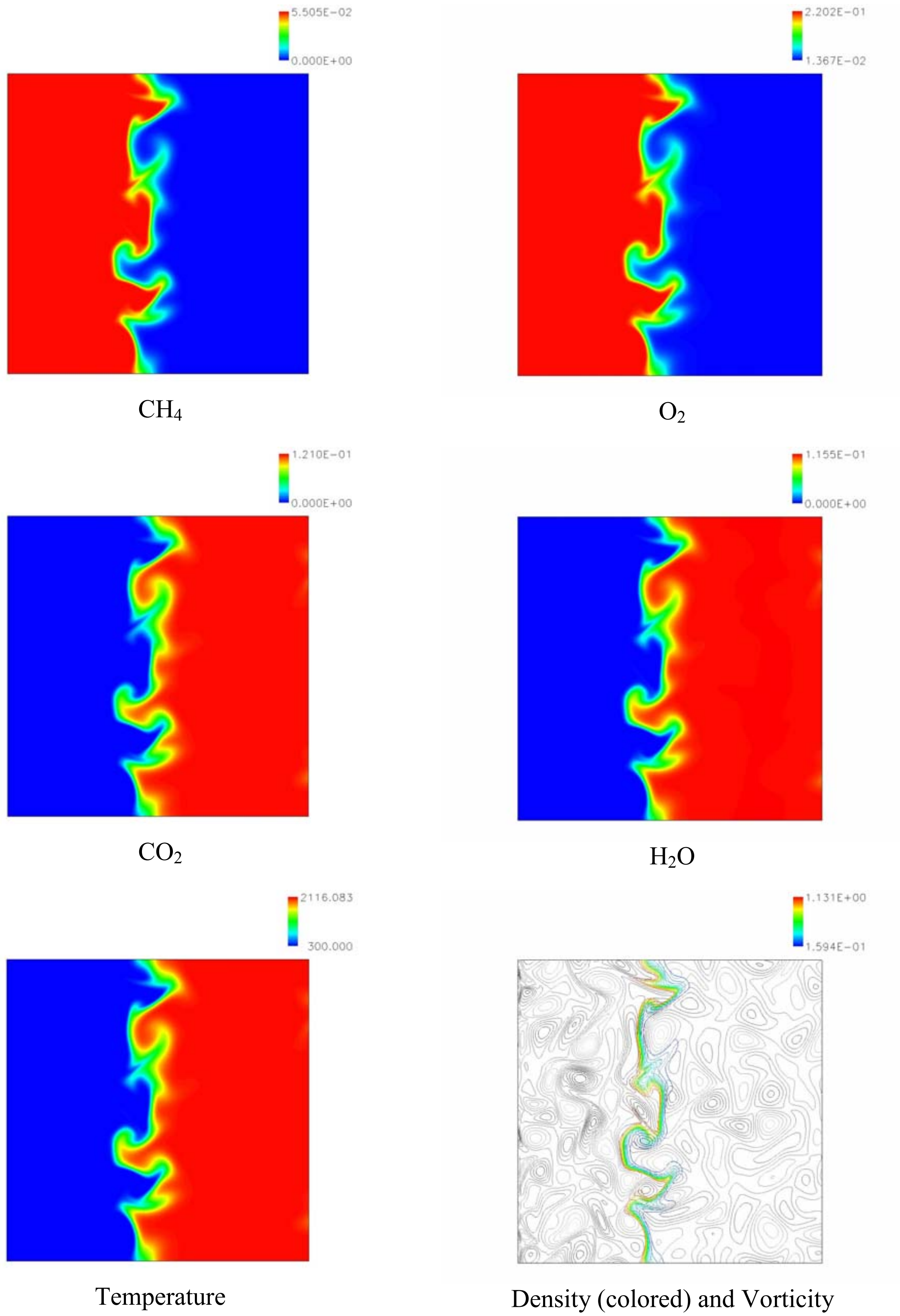


Figure 9. Interaction Between Flame and Turbulence (ANN Results)

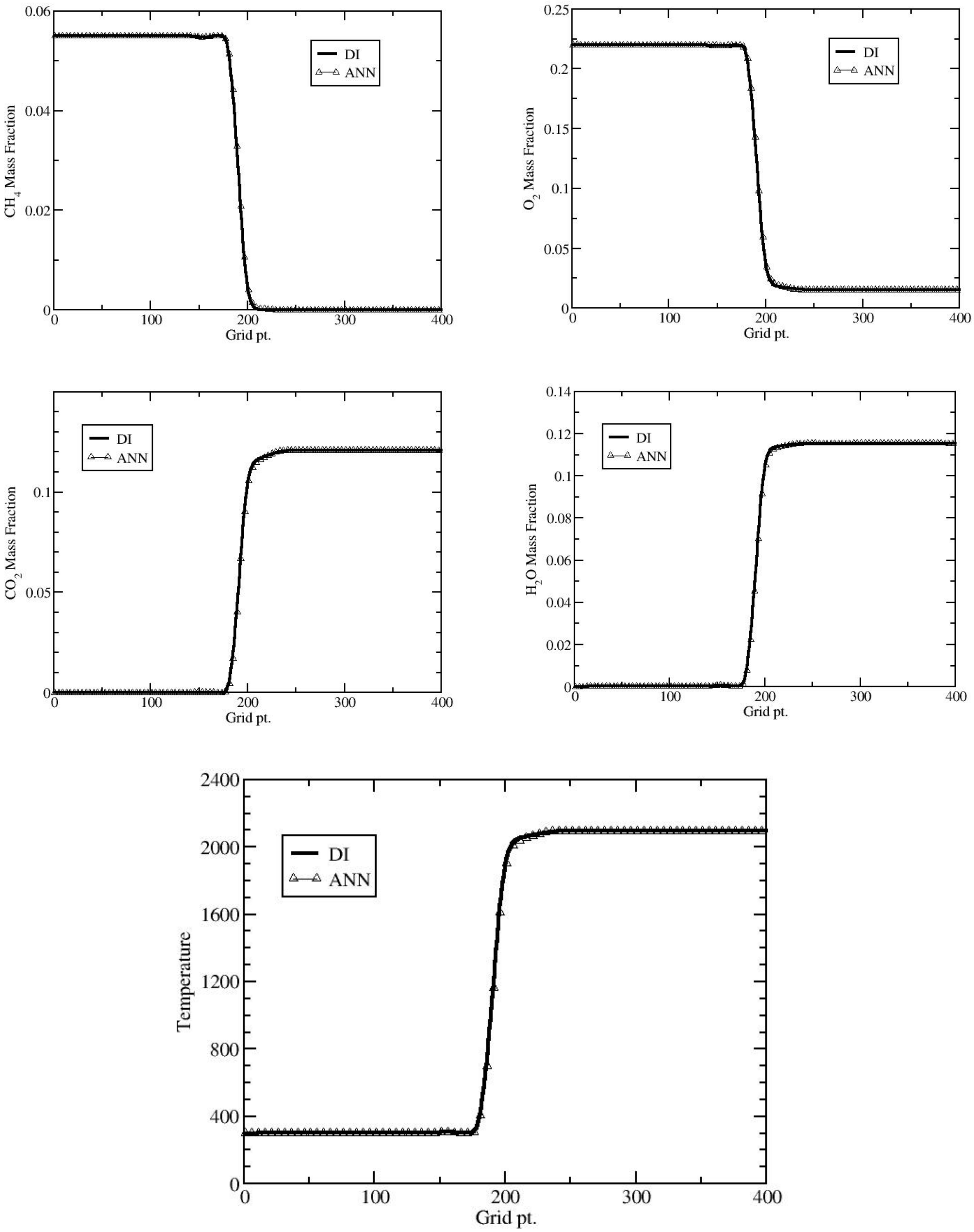
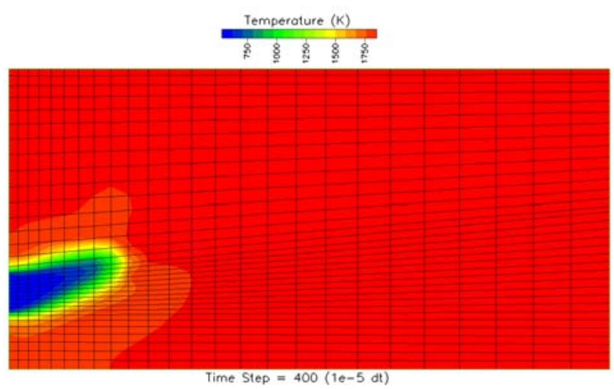


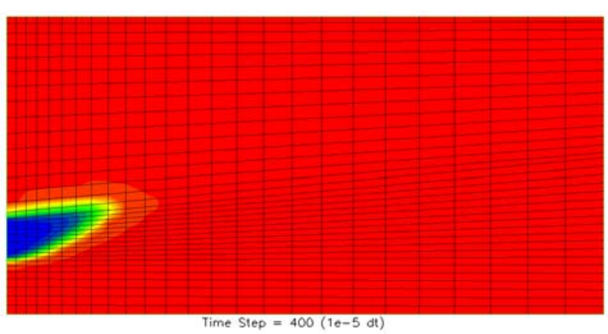
Figure 10. Comparison of DI and ANN Results in the 2D DNS Turbulent Flame

ANN Implementation in CFD-ACE+

The ANN developed by Georgia Tech was implemented and tested in CFD-ACE+. The ANN has been tested for unsteady RANS calculations at conditions of the baseline DOE NETL SimVal combustor (PHI=0.6, Vnoz=45 m/s, Swirl Angle = 45, P = 5.1 atm, Tin = 533 K, Twall = 700 K). A coarse grid simulation was first performed. Figure 11 shows the predicted temperature contours using direct integration and the ANN after 400 timesteps. The transient calculations used a time step of 1e-5 seconds and operator splitting, where reaction rate source terms were computed only once per time-step (i.e. staggered chemistry approach). The results show relatively good agreement between the direct integration and ANN. The ANN flame zone is slightly thinner than the direct integration flame zone. A potential reason for the discrepancy could be due to the different treatment of the reaction rate source term between the ANN and direct integration. For direct integration, the CFD-ACE+ code performs constant temperature reaction integrations. This allows for more robust convergence of the species transport equations. The ANN was generated with Georgia Tech's combustion code, where the temperature is allowed to change during the integrated reaction increment. The changing temperature would enhance the reaction rate slightly during the integration increment. The use of a log transformation of the output was needed to produce accurate ANN results. Previous ANN implementation without the transformation produced poor results for this same case, as the premixture immediately burned at the inlet boundary. Now with the new ANN, the unburned mixture extends 7-8 computational cells into the combustor as expected.



Direct Integration 1-Step Chemistry



ANN 1-Step Chemistry

Figure 11. Predicted Temperature Contours for Coarse Grid Test Case Using Direct Integration and ANN

The ANN was also tested on a finer grid case for the DOE SimVal baseline geometry. Transient calculations were performed for 20,000 timesteps (dt = 1e-5 seconds). These initial results showed a speed-up of 20% for the ANN case compared to the direct integration. This speed-up should increase dramatically for the more expensive multi-step chemistry.

4.5 Premixed SimVal Combustor Case

Georgia Tech performed calculations of the premixed SimVal combustor using their LES code. The grid used is shown in Figure 12. The inflow pipe, combustion chamber and outflow pipe are included in the geometry. The grid mesh is 498x96. A convergent-divergent nozzle is located at the end of the outflow pipe in order to reach outflow supersonic conditions. The numerical scheme used is second order in space and in time. The inflow conditions were provided by the CFDRC to mimic CFDRC's calculations reported last quarter. Supersonic conditions are reached at the outflow of the computational domain. Premixed combustion using the thin-flame model (the G-equation model) is carried out. A turbulent flame speed model is used to represent the flame propagation in this flow.

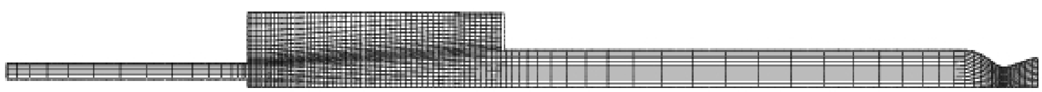


Figure 12. Computational Mesh

Computations without swirl correction:

Figure 13 shows a typical snapshot of the flame location inside the combustion chamber. As far as flow characteristics are concerned, we notice the presence of a re-circulation region created by the expansion of the inlet pipe inside the combustion chamber. Furthermore, due to the abrupt expansion and the separation of the boundary layer at the dump plane, vortices are formed and shed at the dump plane. These vortices undergo pairing and merging process and grow in size such that they become comparable to the dump radius. The flame is located along the interface of these large structures.

For this case without swirl correction, a large amount of fuel escape into the outflow duct before being consumed. Thus, combustion continues in the outflow duct.

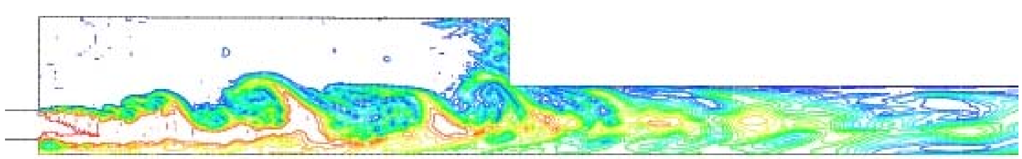


Figure 13. Scalar Field (Red: unburned gas, Blue: burned gas) With No Swirl Correction

Computations with swirl correction:

To account for the swirl component of the flow, we solve an additional equation for third velocity component. However, all terms that are function of azimuthal location are neglected.

Figure 14 shows a typical flame location and flow characteristics inside the combustion chamber. Inclusion of swirl reduces the flame size as expected and the flame is now confined in the combustion chamber. Furthermore, no fuel is present at the centerline and it appears that nearly all fuel is burnt before the flow exits the combustion chamber. These preliminary results confirm that the implementation of the swirl correction into the axisymmetric code is performing as expected.

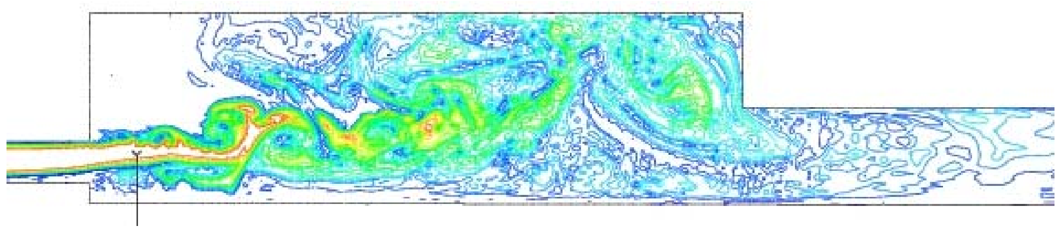


Figure 14. Scalar Field (Red: unburned gas, Blue: burned gas) With Swirl Correction

Combustor dynamics:

At present, the simulation without swirl correction has been completed but the simulation with swirl correction is still underway. Therefore, the pressure spectra and frequency analysis for the latter case still remains to be performed. For the no-swirl case, the pressure fluctuations (Figure 15) inside the combustion chamber are large (the fluctuations from peak to peak represents 20 percent of the pressure mean value). These large fluctuations can force the flame to oscillate, i.e., the flame is alternatively pushed inside the outlet and pushed back inside the inlet. The frequency of the pressure oscillation is 60 Hertz (Figure 16). This mode appears to be related to the bulk (i.e., Helmholtz) mode of the combustion chamber and suggests that without swirl, the flow field does not respond to the longitudinal modes of the combustor or to the mode in the outlet duct. We believe that with inlet swirl and drastic reduction in the flame length that accompanies the swirl, the pressure dynamics in this combustor will switch to the longitudinal mode of this combustor. The present simulation should show this result once it is completed. We will report on this in the near future.

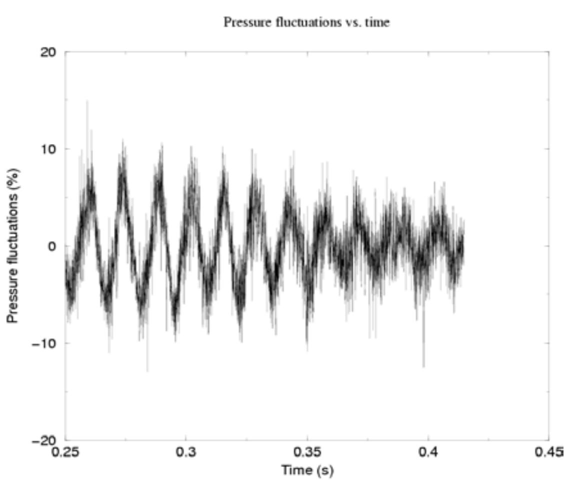


Figure 15. Pressure Time Trace Without Swirl

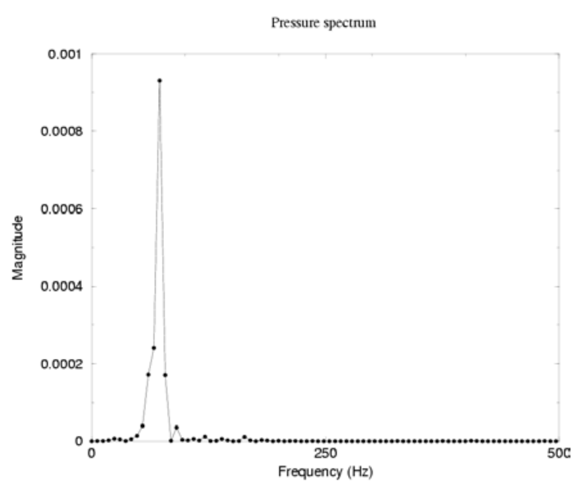


Figure 16. Pressure Spectrum Without Swirl

Future Plans

Georgia Tech will perform simulations with the swirl correction and will be reported next quarter. Also, the DOE-HAT case will be revisited using a flamelet model to predict the effect of combustion on emissions. Turbulent ANN will be used for this purpose.

4.6 Lean Premixed Bluff-Body Combustor Test Case

Detailed temperature and emissions measurements from the Vanderbilt/Sandia (Nandula et al., 1996) lean premixed bluff-body combustor are being used to validate the combustion LES software. This test case was chosen by the industrial consortium during the 2nd consortium meeting at CFDRC in January 2002. The combustion chamber, shown in Figure 17, was configured such that a stainless steel conical bluff body was mounted coaxially at the center of the combustor and served as a flameholder. Flat quartz windows were mounted on the laser receiving side of the chamber and high temperature resistant fiberfrax walls with small holes were mounted on the opposite side.

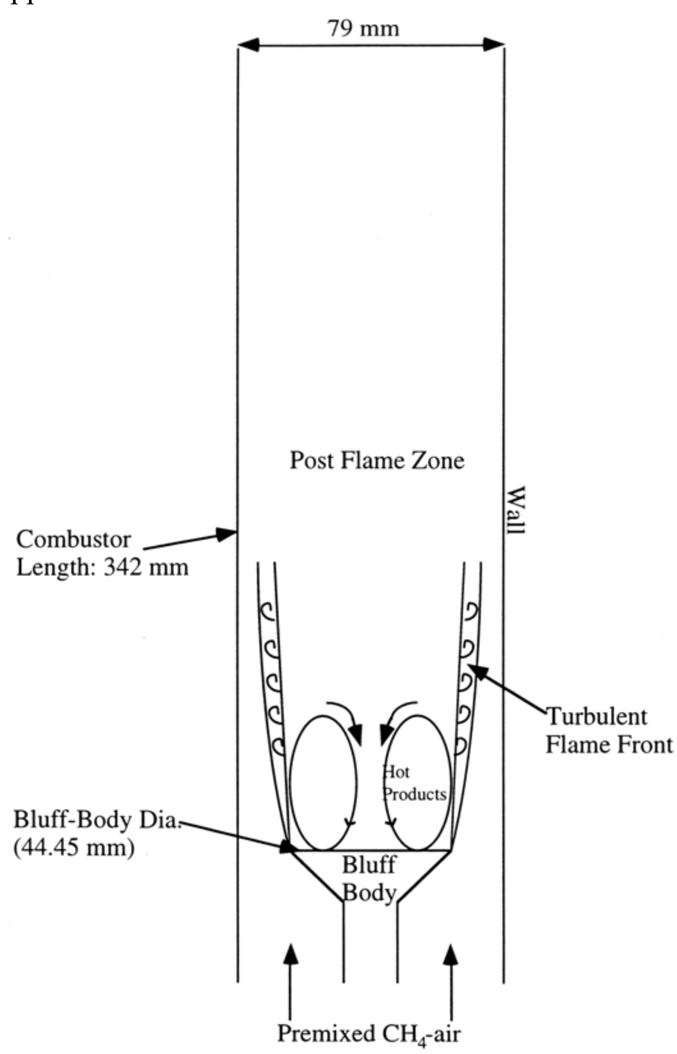


Figure 17. Schematic and Turbulent Flame Structure of Bluff-body-Stabilized Lean Premixed Combustor (Nandula et al., 1996)

The mass flow rate for the bluff-body combustor model was specified by using the measured values reported for the air (3960 SLPM) and the CH4 fuel (244 SLPM). This corresponded to an equivalence ratio of 0.586. The velocity at the inlet to the combustor model, just downstream of a turbulence grid was 15 m/s. An inlet temperature of 300 K and a combustor pressure of 1 atm were also specified. A bluff-body wall temperature of 500 K was used in the simulations and a fixed pressure boundary was used at the outlet.

These initial calculations have utilized the localized dynamic subgrid kinetic energy model (LDKM) for subgrid turbulence with 1-step chemistry and Linear Eddy Mixing (LEM) model for subgrid chemistry. The first calculations using the standard rates from the 1-step chemistry model showed that blow-off occurred. To prevent blowoff, the reaction rates were increased by an order of magnitude and calculations were repeated. Figure 18 shows instantaneous snapshots of temperature, along with the mean temperature. Figure 19 shows a comparison of mean temperature predictions with measurements. Overall good agreement was obtained. As an indication of the difficulty in obtaining good agreement, previous computed mean temperature profiles using 5-step Monte Carlo PDF calculations are shown (Cannon 1997) in Figure 20. The previous Monte Carlo calculations did not capture the enhanced mixing at downstream locations.

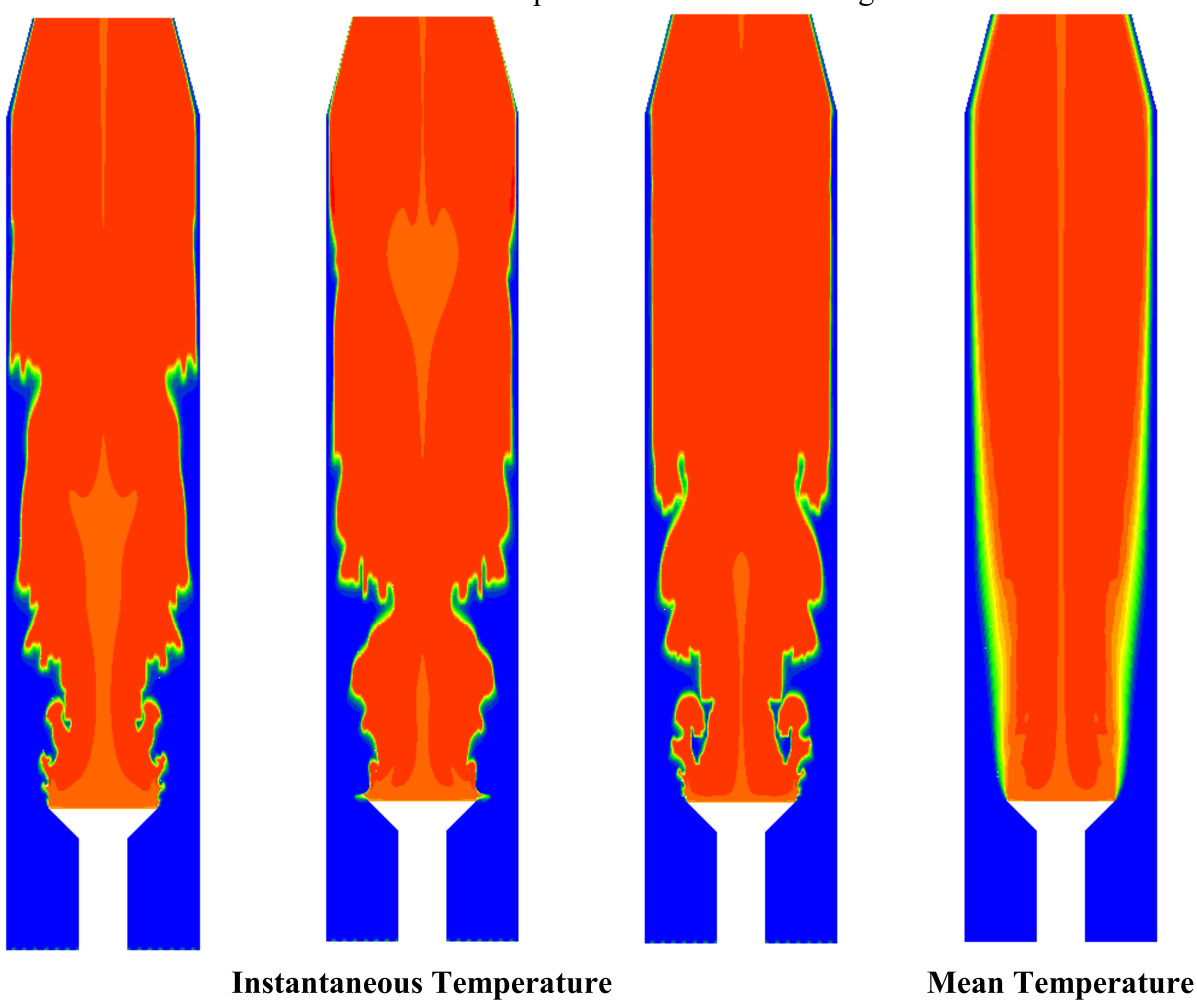


Figure 18. Instantaneous and Mean Temperature Predictions of Lean Premixed Bluff-Body Combustor Using Linear Eddy Mixing (LEM) Model with LES

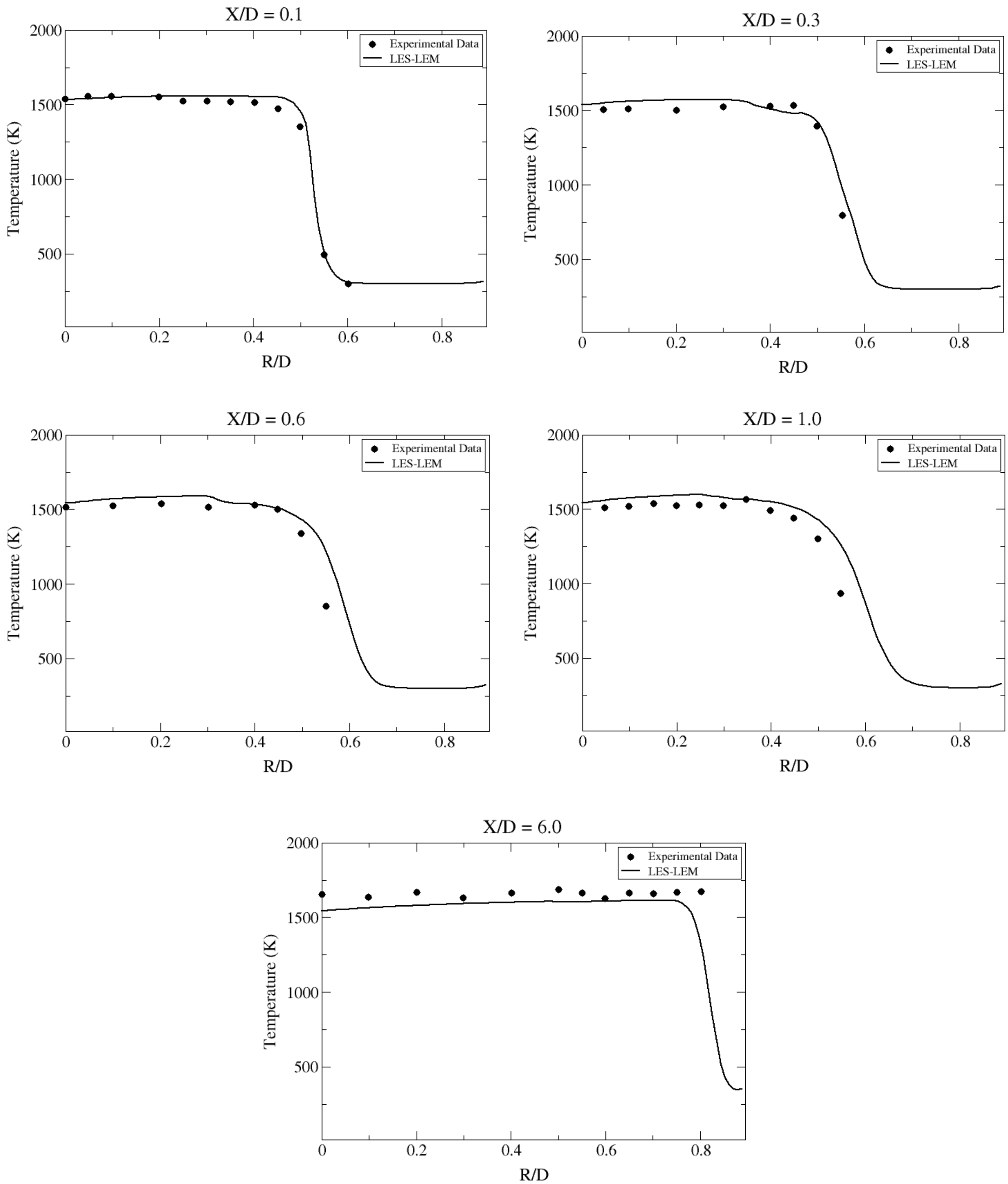


Figure 19. Comparisons of Mean Temperature Predictions and Measurements at Various Axial Locations

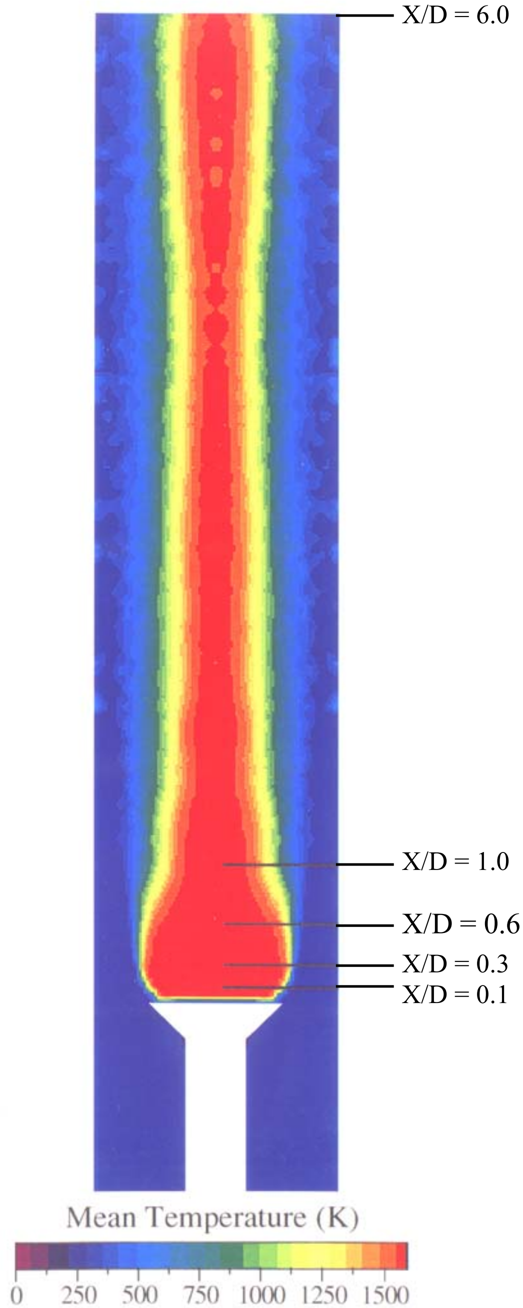


Figure 20. Predicted Mean Temperature in Lean Premixed Bluff-Body Combustor Using 5-step Chemistry and Monte Carlo PDF Method (Cannon, 1997)

As described in section 4.2, the LEM is being modified to more accurately model subgrid turbulence-chemistry interactions. These modifications should improve the predictions and not require ad-hoc increases to the chemical kinetic rates. In addition, 5-step and 15-step chemistry will be utilized in the LEM bluff-body model and will be reported next quarter.

4.7 2nd Industrial Consortium Meeting

The second meeting of the Combustion LES Consortium was held January 31 – February 1, 2002, at CFD Research Corporation (CFDRC) in Huntsville, Alabama. Advanced combustion Large Eddy Simulation (LES) software is being developed under Department of Energy (DOE) and Air Force-sponsored programs. These programs support the development of revolutionary software that can more accurately model turbulent combustion needed to design/analyze advanced low emissions and high performance combustion systems. The three-year development schedule calls for: 1) code development in Year 1, 2) code validation (alpha testing by CFDRC) in Year 2, and 3) code application (beta testing by consortium members) in Year 3. CFDRC has recently completed code development, and is starting on code validation.

A consortium was organized to guide and direct software development/validation, and to provide a means of transferring the combustion LES technology to industry. Twenty organizations are members of the consortium. The organizations represent a cross-section of the combustion community, including representatives of gas turbine combustion (both industrial and aero), burner/boiler manufacturers, fuel injector manufacturers, universities, and governmental agencies. At the second meeting, 18 organizations were represented. Attendees were: M.S. Anand from Rolls Royce, Jurgen Schumacher from Honeywell, Mel Noble and Alan Kubasco from Solar, Paul Matys from Coen, Alan Sayre from McDermott Technologies, Jeff Lovett from Pratt & Whitney, Erlendur Steinthorsson from Parker Hannifin, Shiva Srinivasan from GE Power Systems, George Kalinovich from Woodward FST, Thanh Tran from Vapor Power, Carol Schnepper from John Zink, Dan Maloney and David Huckaby from DOE-NETL, Balu Sekar from Air Force Research Laboratory, Suresh Menon from Georgia Tech, Prateep Chatterjee from Virginia Tech, Marvin Rocker from NASA MSFC, Jamey Condevaux from Williams Int., and Steve Cannon, Virgil Adumitroaie, Keith McDaniel, Scott Crocker, Baifang Zuo, and Cliff Smith from CFDRC.

The first part of the meeting consisted of presentations by the CFDRC team describing their progress in implementing advanced models and solution methods into the existing unstructured, compressible CFD-ACE+ code. Highlights of the presentations were:

1. Reduced chemistry models (5-20 species) have been developed for the following fuels: natural gas, propane, hydrogen, syngas, and JP8. These reduced models were developed from full kinetic mechanisms using the CARM code developed by J.Y. Chen of University of California, Berkeley. These models have been implemented into CFD-ACE+ and tested.

2. In Situ Adaptive Tabulation (ISAT) methods, developed by Pope, have been implemented into CFD-ACE+. These methods allow for chemistry source terms to be stored and later read from a table, rather than always performing direct integration. Pope reports computational speedup factors of 10-50 using ISAT compared to direct numerical integration. To date, CFD-ACE+ has only realized speedup factors of four. A number of modifications have been identified that should improve the computational efficiency, including a better method of calculating the mapping gradient matrix and a better table tree structure (P-K instead of the BSP).

3. Suresh Menon reported on the progress made in developing artificial neural nets (ANN). An ANN for 1-step CH4-Air chemistry was trained at two different turbulent flame conditions (F1 and F3) in a 1-D Linear Eddy flame zone code. The ANN was then successfully used to predict a F2 turbulent flame. The ANN approach is being further developed for the more detailed chemical mechanisms.
4. A 64 PC Beowulf cluster was built from scratch, costing about $1000 per PC. The PC cluster performs at the speed of a supercomputer, at a tenth of the cost.
5. Parallelization of the code has been dramatically improved. Tests were performed that show 80% computational efficiency on a Beowulf cluster of 64 PCs when running a 3.5M cell LES case.
6. The Linear Eddy Mixing (LEM) model, developed by Suresh Menon at Georgia Tech, was implemented and tested. LEM models the subgrid turbulence-combustion interaction in LES calculations, and is an essential model to accurately calculate turbulent combustion. The LEM model was shown to agree well with the measurements of a premixed reacting backstep experiment, while other steady-state, unsteady RANS, and LES with laminar chemistry calculations did not.
7. Spray tracking and atomization models have been implemented and tested. Future work includes implementing a multi-component vaporization model to allow the use of the reduced (20 species) JP8 mechanism, and a supercritical vaporization model (being developed by the University of Wisconsin – Madison).

Everyone seemed impressed with the development to date.

After these presentations, Dan Maloney discussed the DOE-NETL SimVal experiment that will be performed starting this summer and running for a number of years. This experiment will provide extensive measurements to be used for code validation of turbulent reacting flows at realistic gas turbine conditions. The experimental geometry will have hard (choked) acoustic boundaries at both the inlet and exit to establish the full computational domain. Measurements will consist of high response pressure measurements, flame visualization, exit emissions, lean blowout, etc. The experiment is constructed so as to systematically change various parameters that might affect instability and emissions. DOE will make the measurements available to the public, and are hopeful that the measurements will become a benchmark for CFD validation of turbulent reacting flows.

Steve Cannon of CFDRC then presented preliminary predictions of the DOE-NETL SimVal experiment. These predictions were performed using 2D URANS and LES methods, realizing that 3D computations will follow in the future. The baseline case showed a 400-hertz instability. The premix barrel length was shown to have a substantial effect on pressure oscillation amplitude and frequency. The effect of eliminating the downstream resonant section and replacing it with an increased combustor section was also studied. Finally, the effect of equivalence ratio on instability was presented.

<u>Validation Cases</u>

On the second day, the focus shifted to what validation cases should be run by CFDRC during alpha testing. Funding is available to perform four validation cases. Steve Cannon presented a number of potential validation cases, and then the consortium members broke into three work groups to assess the cases and list what cases they desired. The three work groups consisted of: 1) burner/boiler manufacturers, 2) industrial gas turbines, and 3) aero/liquid fuel gas turbines. The burner/boiler manufacturers stated they wanted the following cases: 1) Bluff-body experiment of Vanderbilt, 2) Tecflam experiment, 3) Weak-swirl experiment from Berkeley. It was assumed that the DOE-NETL SimVal experiment would also be one of the four cases studied. This group also expressed the desire to be able to accurately predict emissions (NO_x, CO, OH), temperature profiles, gaseous radiation, flame instability, and burner-to-burner interaction.

The industrial gas turbine group assigned the following cases to their want list: 1) GE LM6000 case, 2) P&W Dry Hat experiment (tested at DOE), and 3) Solar Taurus 70 case. Once again, the DOE-NETL SimVal case was assumed to be one of the cases that would be studied. It is unsure if the data from the first three cases are in the public domain. Consortium members (Shiva Srinivasan, Dan Maloney, and Mel Noble) were asked to check on the public domain issue. Issues important to this group included vortex shedding from fuel spokes, fuel-air distribution at the end of the fuel injector, premixedness, and heat flux to the liner.

The aero/liquid fuel group did not decide on four cases, but instead listed approximately fourteen cases, ranging from diffuser flows, non-swirling and swirling jets and flames, swirling recirculating flames, premixed combustor, and flames with sound measurements. Other cases they mentioned were a spray data-set from Parker, NASA Host data, P&W data for combustion instability, and gas-gas co-axial rocket injector data. Unfortunately, this group did not come up with a succinct list.

The recommendations of the work groups will be taken into consideration, and a final list of validation cases will be selected by CFDRC.

Consortium Funding

The final item discussed at the consortium meeting was how to spend the $150K of consortium money given by consortium members to improve the combustion LES software. Three areas need further development: 1) an improved gaseous radiation model, 2) post-processing software for combustion LES and general combustion analysis, and 3) new atomization models (e.g. airblast atomization). After discussing these tasks, the consortium members who contributed to the consortium funding voted on which tasks they preferred. No consensus was reached. CFDRC will decide which tasks to fund, once other funding opportunities have been decided.

Next Combustion LES Consortium Meeting

The next meeting will be held in October or November 2002 at CFDRC. Comparisons of combustion LES predictions and measurements will be made for the four cases selected. After the meeting, a two-day training class will be held for the beta testers. Approximately eight organizations will take part in beta testing.

5. CONCLUSION

The combustion LES code has been further developed and tested for predicting turbulent reacting flows. The LES code can now use the LEM to better represent turbulent reacting flow since subgrid stirring effects are now resolved. The ISAT has been refined and optimized and gives a 2-3 speedup using the 9 species mechanism derived from the full GRI. The artificial neural net (ANN) approach has been demonstrated in Georgia Tech's single cell LES code but needs to be implemented and tested in CFD-ACE+. The LES code has undergone initial testing with the premixed SimVal baseline combustor.

6. REFERENCES

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Maloney, D., (2002), Personal Communication, DOE-NETL.

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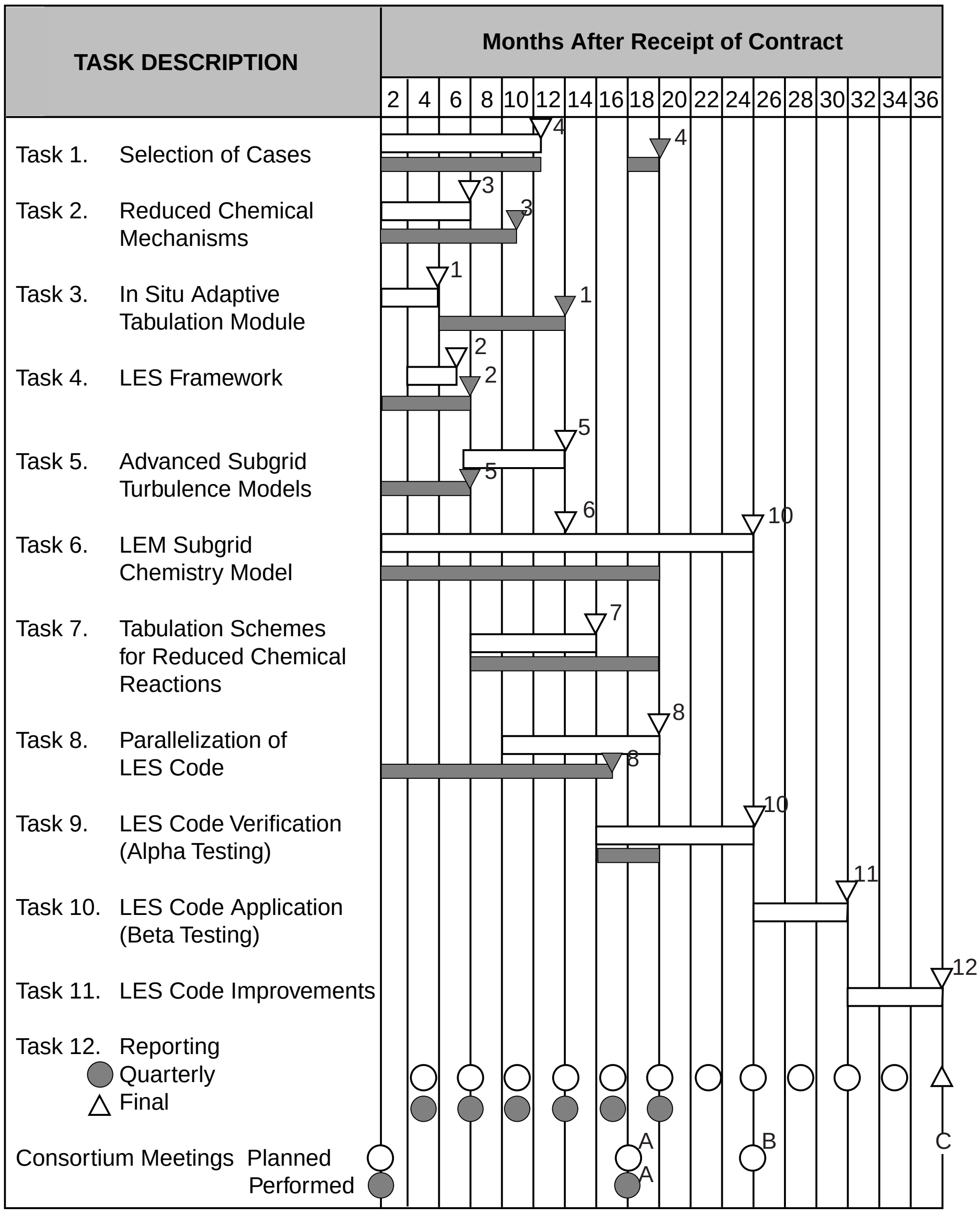
Pitz, R.W. and Daily, J.W., (1983), "Combustion in a Turbulent Mixing Layer Formed at a Rearward-Facing Step," AIAA J. 21 pp.1565 --1570.

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. Optimize and refine ISAT for large chemical mechanisms (> 19 species).

2. Carry out initial validation of LES code for predicting emissions and instability in selecting cases from industrial consortium.

3. Develop, implement, and test neural net on lean premixed SimVal combustor test case.