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

Quarterly Technical Progress Report for

July - September 2002

by

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ABSTRACT

Further development of a combustion Large Eddy Simulation (LES) code for the design of advanced gaseous combustion systems is described in this eighth quarterly report. CFD Research Corporation is developing 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-HAT combustor, the Loughborough University combustor port flow experiment, and the Vanderbilt-Sandia combustor.

Next quarter, LES software development and testing will continue. Alpha testing of the code will continue to be performed on cases of interest to the industrial consortium. Beta testing of the code will also begin, as nine organizations will exercise the LES code on combustion problems of their choice. Training of the beta test site personnel will be done at the third consortium meeting. The consortium meeting will also include presentations on the LES code validation by CFDRC during the past year.

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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) has been utilized to help develop and implement these advanced submodels in the unstructured, parallel CFD flow solver. Efficient numerical algorithms that rely on *in situ* look-up tables or artificial neural networks have been implemented for chemistry calculations. In the second year, the combustion LES software has been evaluated and validated using experimental data from lab-scale and industrial test configurations. During the last year, nine industrial and academic partners will take the combustion LES code and exercise it on problems of their choice. Final feedback and optimizations will then be implemented in the final release version of the combustion LES software.

2. EXECUTIVE SUMMARY

Work in this eighth quarter (July - September 2002) has included further development of the turbulent ANN for LEM subgrid models. Combustor LES validation has been carried out on the DOE-HAT lean premixed combustor, the Loughborough University's combustor port experiment, and the Vanderbilt-Sandia combustor.

Next quarter, completion of the following tasks are planned:

1. Finish DOE-HAT lean premixed combustor validation case.
2. Implement and test TANN on lean premixed SimVal combustor test case.
3. 3rd Combustion LES Consortium Meeting.
4. Train and support beta site testers.

3. EXPERIMENTAL

No experiments were performed this quarter.

4. RESULTS AND DISCUSSION

4.1 Turbulent ANN for Efficient Subgrid LEM

4.1.1 Introduction

A *Laminar Artificial Neural Network (LANN)* has been developed for a reduced-step 9-species mechanism (H_2 , O_2 , OH , H_2O , CH_4 , CO , CO_2 , NO and N_2) and a new *Turbulent Artificial Neural Network (TANN)* has been developed for the single step Westbrook-Dryer mechanism (with 5-species (CH_4 , O_2 , CO_2 , H_2O and N_2)) for methane-air combustion. The ability of these two ANNs is demonstrated using 2D-DNS and LES studies of a stationary flame-turbulence interaction test case.

4.1.2 Discussion

9-species LANN: The present laminar ANN development for the 9-species mechanism is more novel in concept when compared to the previous LANNs. As previously carried out, the training set is evaluated and pre-processed from a different code, which involves a point-evolution of the chemistry given an input set of conditions ($\Phi=1.0$; $T=300\text{K}$, $P=1\text{atm}$). In the previous work, a logarithmic transformation is used for the pre-conditioning of the training sets. However, this time, different transformation functions have been used for each of the individual species and temperature. Some of these are still logarithmic but others are not. This ensures still better quality of ANN training sets. This laminar ANN is tested on a 2D DNS code, and the results are compared with those for the same problem using direct integration (DI). The training set for the ANN is chosen from this setup. As previously, the advantage of choosing the training set this way is that it has considerably reduced the total number of sample points taken for the ANN training, thus making the process faster. Also the points are picked up in a much efficient manner since it eliminates any biasing of the sample points in any temperature range.

LANN for the reduced-step 9-species methane-air mechanism is developed using this concept. Figure 1 show some instantaneous contours of CH_4 and temperature. Figure 2 shows some instantaneous contours for the pollutants. Figure 3 shows the time-averaged profiles as obtained from LANN versus a direct integration simulation for the same case.

CH₄

Temperature

Figure 1. Instantaneous Profiles Using 9-species LANN

CO

NO

Figure 2. Instantaneous Profiles Using 9-species LANN

Figure 3. Scalar Profiles for Species/Temperature (ANN v/s DI) for the 9-species LANN

Figure 3 (concluded). Scalar Profiles for Species/Temperature (ANN v/s DI) for the 9-species LANN

5-species TANN: The concept of a laminar net is further extended to bring in the effect of turbulence effects in the flow. Almost all practical combustor applications require incorporation of turbulence effect on the reaction rate (i.e., the filtered reaction rate need to be obtained). This implies that intricate coupling between the chemical rates and the turbulence length and time scale parameters must be incorporated. A turbulent artificial neural network is developed for this purpose. This TANN can mimic the effect of the local turbulence parameters on the chemical reaction rates for combustion. The mass fractions of the involved scalars and the temperature are input parameters to both LANN and TANN. However, in addition for TANN, we have introduced the local turbulence fluctuation (u') and a corresponding length scale (l) as two new input parameters. The TANN training set is obtained from fine-resolution DNS simulations of flame-turbulence interactions in a 2D domain. The overall chemical rates are stored as a function of the turbulence eddy and the local rms fluctuation (in addition to the scalar and temperature inputs). Since the most practical application of the TANN is for engineering LES, where we are interested for the subgrid scale effect on the reaction rates, a spatial filter and local time-averaging are performed before training. The approach for the development of the TANNs are similar to the LANN development: discretized binning of the dataset for optimal training, preconditioning of the data-set (using logarithmic transformation), etc. Parallel concepts for discretization of the network, on the basis of u' and/or l are to be explored in the future. Figure 4 show some instantaneous comparisons for the fine-resolution DNS runs and the corresponding coarse-grid runs using TANN. As can be seen from the figures, the TANN is able to capture the overall flame-turbulence behavior, however the small-scale effects are not captured very well. However, this is to be expected since the TANN-LES is carried out on a much coarser grid (100x100) compared to the DNS (400x400). Direct comparison of instantaneous images is also not possible since the time step for LES is much larger than for the DNS. We are currently evaluating these results from statistical point of view to make more quantitative comparison.

4.1.3 Conclusions

A new 9-species LANN for a methane-air mechanism is developed. The main advantage this network offers is its ability to predict the two most significant pollutant emissions (CO and NO). This is a significant development since this result suggests that LANN for even more complex kinetics (e.g., 19-species) can be developed. This will be investigated very soon. The new TANN model is more robust than the previous attempt and its application in a LES shows its ability to capture the resolved-scale wrinkling of a turbulent flame. Future plans are to develop the TANN for the 9-species and to apply it to three test cases (a) flame-turbulence interaction problem used earlier, (b) the Sim-Val test combustor (DOE new combustor) and a bluff-body and swirl stabilized non-premixed flame recently studied by Masri.

Figure 4. Instantaneous Species and Temperature Profiles Using 5-species TANN-LES (right) Compared to DNS (left) Results

CO₂

H₂O

Temperature

Figure 4 (concluded). Instantaneous Species and Temperature Profiles Using 5-species TANN-LES (right) Compared to DNS (left) Results

4.2 Combustor Port Flow Validation Case

Experimental data from a combustor port flow at Loughborough University is being used for validation of the combustion LES code. Adrian Spencer, assistant professor at Loughborough University, was responsible for acquiring the data and was recently at CFDRC doing the validation work. Initial results were presented last quarter. More detailed results are presented here to show the improvement of LES vs. RANS for jet-in-crossflow modeling.

The test case is comprised of two concentric pipes. The inner pipe has a row of 6 equi-spaced ports which allows flow from the annulus feed to enter the inner pipe, or core, see Figure 5. By using various valves it is possible to set the following parameters; jet Reynolds number, annulus bleed flow fraction and jet to core flow velocity ratio. These three bulk flow parameters fully define the test condition, and may be varied to represent primary zone or dilution zone type port flows. Measurements of an impinging flow are available for a jet to cross flow ratio of 5 and an annulus bleed flow of 50%, with a jet Reynolds number of around 24000. It is this case that was simulated using LES and RANS.

Figure 5. Co-Ordinate System Used for the Test Section

The set-up and boundary conditions were described in the previous quarterly report. The grid density was chosen based on previous RANS grid refinement studies. It was found that 100,000 cells for a grid independent RANS calculation required 2,200,000 cells for a full 3D LES study at a similar grid density. Here, in Figure 6, a butterfly grid is used in the core and an O-grid in the annulus. Each port contains 15x15x5 cells connecting the core and annulus domains. The LES modeling utilized the Smagorinsky model for subgrid turbulence and a time-step of 2.5e-4 seconds. The calculations were performed on CFDRC's 16 PC Linux cluster.

Figure 6. Surface Grid

Figure 7 shows one instantaneous snapshot of the velocity vectors in-line with the jets. The velocity vectors are colored by a passive scalar to indicate the origin of the fluid. It can be observed that the jet fluid penetrates a significant distance upstream of the ports. This upstream penetration is in agreement with experimental data as indicated by the block x. Random turbulent structures are observed throughout the flowfield.

Figure 7. Instantaneous LES Snapshot of Combustor Port Flow

A comparison of predicted and measured mean velocity profiles are shown in Figure 8. The radial profile location is indicated in the velocity vector plot. Here it can be seen that LES is much better at capturing the higher negative u-velocity on the centerline compared to RANS. It is likely that the symmetric nature of the RANS calculation prevents the back-and-forth movement of flow about the combustor centerline. This movement about the centerline, as captured with LES, is needed to predict the higher backflow rates.

Figure 8. Comparison of Measured and Predicted Profiles of Mean U and V-Velocity in Combustor Port Flow

A comparison of RMS velocity results are shown in Figure 9. Here, it is clear that the RANS greatly under predicts the rms levels of both the U- and V-components. LES does a much better job at predicting the rms values. Some discrepancies do exist along the shear layer of the jet up near the port where higher frequency vortices were observed experimentally. These high frequency vortices were not captured with the LES and would require more grid resolution. These smaller structures don't seem to have a large impact on the mean flowfield.

Figure 9. Comparison of Measured and Predicted Profiles of rms U and V -Velocity in Combustor Port Flow

The predicted and measured U -velocity PDF is shown in Figure 10 at the upstream penetration location at the centerline. The LES does a good job of predicting the velocity PDF. Possibly more timesteps are needed to smooth out the PDF since only 2 seconds of data have been used (versus 82 seconds for the experiments). The LDKM model is presently running and may capture the smaller eddies in the jet shear layer near the orifice. Overall, the LES with Smagorinsky has produced good results, showing significant improvements over steady RANS analysis.

Figure 10. Comparison of Measured and Predicted U-PDF at Upstream, Centerline Location

4.3 DOE-HAT Combustor Validation Case

The DOE-HAT combustor configuration was modeled and comparisons to experimental CO and NO_x measurements were performed. The DOE-HAT combustor was studied in an experimental program at DOE-NETL in Morgantown, WV in collaboration with UTRC. Experiments were performed at lean conditions over a range of equivalence ratio, pressure, and moisture level. Also, two different nozzle configurations were studied. For the validation simulations performed here, only the equivalence ratio and pressure will be varied. The calculations will be performed with dry reactants and with one particular nozzle. The nozzle consists of an axial swirler and fuel spoke downstream of the swirler. The nozzle flow dumps into a cylindrical refractory-lined combustor. A 3-hole water-cooled suction probe is situated downstream in the combustor to provide CO and NO_x measurements.

4.3.1 Steady RANS Detailed Nozzle Calculations

Steady-state calculations were first performed on a 1/16th sector of the nozzle to predict the fuel flow through the spoke and out into the air stream within the nozzle. Then the predicted exit profiles of velocity, pressure, temperature, turbulence quantities, and equivalence ratio were mapped to a full 3D combustor geometry as an inlet. This boundary condition mapping prevents extremely large grid counts that would be needed to model all 15 swirl vanes and fuel spokes. It was found that the mixing was strong enough in the nozzle to achieve a tangential uniformity before dumping into the combustor. However, there were significant radial gradients at the nozzle exit that could only be predicted with the full swirl vane/spoke geometry.

The swirl vane/fuel spoke geometry is shown in Figure 11. The geometry is rotated and copied to show 3 vanes and 3 spokes. This detailed steady-state modeling of the nozzle required ~1 million cells and was performed on a 14 PC cluster. Domain decomposition was performed normal to the x-direction in such a manner that identical cyclic faces were maintained on each processor. A many-to-one grid interface was utilized within the combustor to enable coarser cells in the downstream section of the combustor. The following flow conditions were modeled in the initial baseline case:

$T_{\text{inlet}} = 734 \text{ K (862 } ^\circ\text{F)}$
 $P_{\text{comb}} = 200 \text{ psia (13.6 atm)}$
 $m_{\text{air}} = 0.96 \text{ kg/sec (2.116 lbm/sec)}$
 $\text{PHI} = 0.54 \text{ (CH}_4\text{-air); 0.58 (natural gas-air)}$
 $\text{Nozzle_ACD} = 12.3 \text{ cm}^2 \text{ (0.79 in}^2\text{)}$

Figure 11. Velocity Magnitude Contour (140 m/s) Colored with PHI for Full Swirler Vane/Fuel Spoke Geometry

Fixed mass flow boundaries for air and methane were assumed upstream of the swirl vane and fuel spoke manifold respectively. Fuel jet velocities near 230 m/s were predicted through the fuel orifices and an ~18% pressure drop was predicted through each fuel orifice. The OD of the fuel nozzle was 2.48" and the ID was 1.38". The combustor diameter was 4.25". CO and NOx measurements were provided from a 3-hole probe at a 15" location downstream of the fuel nozzle.

The predicted results along a radial-axial plane from the detailed swirl-vane/fuel spoke geometry are shown in Figure 12. These results were obtained from similar conditions to the baseline, except that the equivalence ratio was leaner at a value of 0.5 (natural gas-air). These results show that higher axial and tangential velocities are formed along the OD of the nozzle. This is due to the lower blockage from the swirler and fuel spoke along the nozzle OD. The higher axial velocities on the OD create leaner mixtures on the OD. This lean OD mixture results in a relatively lean region along the combustor OD. The equivalence ratio in the combustor outer recirculation zone is ~0.35. The central recirculation zone equivalence ratio is ~0.6.

Figure 12. Axial-Radial Planes of Axial and Tangential Velocity, Equivalence Ratio, and Total Pressure

Figure 13 shows the radial-tangential planes of predicted equivalence ratio, total pressure, and axial velocity near the nozzle exit. These results clearly show the tangential uniformity achieved near the nozzle exit. This allowed for a simplified radial profile boundary condition mapping to the full 3D combustor geometry used in the LES calculations.

Figure 13. Predicted Radial-Tangential Planes of Axial Velocity, Total Pressure, and Equivalence Ratio $\frac{1}{2}$ " Upstream of OD Nozzle Dump Plane

4.3.2 LES Combustor Calculations

The previously predicted profiles of velocity, equivalence ratio, temperature, pressure, and turbulence kinetic energy were mapped to the full 3D combustor inlet bc. Figure 14 shows the computational domain for the 3D combustor that started $\frac{1}{2}$ " upstream of the nozzle OD dump plane and ended 18.5" downstream of the nozzle dump. A fixed mass inlet was applied and a fixed static pressure was applied at the exit. RMS velocity fluctuations of 10 m/s were applied at the inlet. A many-to-one interface was used part-way down the combustor to coarsen the grid in downstream regions. A total of 1.34 million cells was required. The computational domain was decomposed onto 22 processors and calculations were performed on CFDRC's Linux cluster of 1400 and 1670 MHz AMD Athlon processors.

A partially converged steady-state solution was used as the initial conditions and a time-step of $7.5E-6$ seconds was utilized. The LDKM subgrid turbulence model was used with an assumed pdf method for the subgrid chemistry model. A 2-dimensional PDF with a top-hat and tri-delta shape for the mixture fraction and progress variable was assumed. A 2-step chemical mechanism was used, where the fuel oxidizes to CO and then the CO oxidizes to equilibrium products at finite rates. The thermal NO_x mechanism was included at each time-step by solving a separate transport equation for NO_x. The influence of mixture fraction and progress variable fluctuations were included in the mean NO_x and CO rates.

Figure 14. Computational Domain and Grid for 3D LES of the DOE-HAT Combustor

Instantaneous and mean snapshots of predicted flow-field variables are shown in Figure 15. The dark solid line at the downstream end of the combustor represents the 15" mark where comparisons to measurements are made. It will be interesting to run a steady-state RANS calculation to convergence to determine the flowfield differences for this reacting swirling flow case. First, it is clear that more time-steps are needed to obtain enough statistics. The non-symmetric nature of the mean flowfield would indicate this. Also, the case has only been run 1.75 flow-through times, with statistics collection taking place for only the last 0.75 of a flow-through time.

These results show that random and coherent structures are captured in the instantaneous snapshots. The temperature contours indicate high-frequency vortex structures forming in the outer shear layer. The leaner fuel-air mixture from the nozzle OD flow is maintained $\frac{3}{4}$ of the way down the combustor outer wall. This lean flowfield produces low CO and NO_x emissions near the combustor wall at the 15" downstream location. The core of the flow shows significant CO formation in the upstream section of the combustor in the flame zone near the shear layers. Oxidation occurs down to levels of around 40 ppm, just slightly above equilibrium levels (~26 ppm). Peak NO_x levels are observed halfway down the combustor in the core. This is the location of max temperature and equivalence ratio. It is also the location where the flow is relatively stagnant, so long residence times exist. At the downstream 15" location the NO_x levels are also around 40 ppm. Comparisons with measurements are shown in Table 1. The comparisons are good for this baseline case. The predictions are only about 10% lower than the experimentally observed values. Further cases at leaner conditions and at different pressures will be performed. The ability of the model to capture the sharp increase in CO at ultra-lean conditions (PHI=0.42) will be determined and will be reported next quarter.

Figure 15. LES Mean and Instantaneous Flowfield Variables for the Baseline DOE-HAT Combustor Case

Figure 15 (continued). LES Mean and Instantaneous Flowfield Variables for the Baseline DOE-HAT Combustor Case

Figure 15 (continued). LES Mean and Instantaneous Flowfield Variables for the Baseline DOE-HAT Combustor Case

Figure 15 (concluded). LES Mean and Instantaneous Flowfield Variables for the Baseline DOE-HAT Combustor Case

Table 1. CO and NO_x Emissions Data and Predictions for DOE-HAT Baseline Case

	CO (ppm)	NO _x (ppm)
Experimental Data	44.3	41.5
LES Time-Average	38.7	37.7

4.4 Vanderbilt-Sandia Combustor Validation 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 and was described in the last quarterly report. This quarter, the combustor LES calculations were performed with reduced multi-step reaction kinetics (5- and 15-step mechanisms from the full GRI2.11) and with the Linear Eddy Mixing (LEM) subgrid chemistry model. Details of these results were presented at the Natural Gas Technologies conference in Orlando, FL during the month of October. Details of the validation study can be found in the paper included as Appendix C.

5. CONCLUSION

The combustion LES code has been further developed and tested for predicting turbulent reacting flows. The use of a 9-species Laminar Artificial Neural Net (LANN) was successfully demonstrated by Georgia Tech in their 2D DNS Code. The use of Turbulent Artificial Neural Nets (TANN) is still being demonstrated. The accuracy of the combustion LES code was demonstrated with good predictions of the Vanderbilt lean premixed atmospheric combustor, the DOE-HAT high pressure combustor, and the Loughborough University combustor port flow cases. Training of the beta site testers will begin this next quarter at the 3rd Combustion LES Consortium meeting.

6. REFERENCES

Chakravarthy, V.K. and Menon, S., 1999, "Large-Eddy Simulations of Turbulent Premixed Flames in the Flamelet Regime," *Combustion Science and Technology*, Volume 162, pp. 175-222.

APPENDIX A — WORK SCHEDULE

Key Milestones

1 Complete In-Situ Adaptive Tabulation Module	7 Complete Tabulation Schemes
2 Complete LES Framework Modification to CFD-ACE+	8 Complete Parallelization of LES Code
3 Complete Reduced Mechanisms	9 Complete Implementation of LEM Model
4 Complete Selection of Cases	10 Complete Alpha Testing of LES Code
5 Complete Implementation of Turbulence Models	11 Complete Beta Testing of LES Code
6 Complete Implementation of Initial Version of LEM Model	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 Bar] Planned
 [Performed Bar] Performed

APPENDIX B — FUTURE PLANS

During the next quarter, the following work is planned:

1. Train and support beta testers.
2. Continue CFDRC validation of LES code for predicting emissions and instability in selected cases.
3. Test turbulent artificial neural net on lean premixed DOE SimVal combustor test case.

APPENDIX C — LEM BLUFF-BODY VALIDATION PAPER

LINEAR EDDY SUBGRID MODELING OF LEAN PREMIXED METHANE-AIR COMBUSTION

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ABSTRACT

A bluff-body stabilized lean premixed combustor has been numerically studied using Large Eddy Simulation (LES). Available experimental data from Pitz and co-workers at Sandia Labs and Vanderbilt University, including, spatially resolved mean temperature and emissions, were compared to the LES predictions. The combustion LES utilized various subgrid chemistry descriptions including simple 1-step, laminar assumptions to 5-step, Linear Eddy Mixing (LEM) models. The LEM model represents the state-of-the-art in resolving subgrid turbulence-chemistry interactions since it captures molecular mixing and chemical reaction in 1D down to the molecular level and models the unresolved turbulent stirring using Kolmogorov cascade laws. It was shown that the LEM was needed to predict the turbulent reacting bluff-body flow. Laminar chemistry assumptions do not allow large-scale turbulent structures to form and the subsequent enhanced mixing downstream of the bluff-body. 3D modeling was also needed instead of 2D axisymmetric modeling since non-symmetric large scale motion strongly influenced the predictions resulting in better agreement with the data. As computers become continually faster and cheaper, is anticipated that LES with appropriate subgrid chemistry modeling will be used as a routine design tool for natural gas-fired combustion systems in the near future. LES is already being used to solve difficult instability challenges facing the lean premixed gas turbine combustor community.

INTRODUCTION

The ability to predict the behavior of turbulent reacting flow systems is important in the economical design of low-emission gas turbines. Lean premixed combustion offers a practical way of restricting NO_x emissions to less than 10 ppm. In order to efficiently design and optimize such combustors, a reliable comprehensive model that can treat the turbulent fluid flow, heat transfer, chemistry, and their interactions is needed.

Large Eddy Simulation (LES) has been developed to predict the large-scale, energy containing turbulent scales within a given flowfield. Unlike standard computational fluid dynamics (CFD) methods that use steady-state assumptions, LES can capture periodic unsteady mixing, countergradient diffusion, and interactions with natural system acoustics. Models for LES are needed for turbulent mixing below the grid scale (i.e. energy containing scale). These turbulence and chemistry subgrid models are more justified and more widely applicable since subgrid processes are more universal than models needed for steady-state CFD codes.

Adequate subgrid chemistry modeling is crucial since chemical reactions take place at the molecular level, well below the resolution of LES grid sizes for typical combustors. The Linear Eddy Mixing (LEM) model was developed by Kerstein (1992) to resolve chemical reactions and molecular diffusion down to the Kolmogorov scale and model the effects of turbulent stirring at scales smaller than the local LES grid. The LEM can handle multi-step chemical reactions and can resolve turbulent mixing interactions for a range of time scales including the fast intermediate radical reactions and the slower NO_x producing reactions.

Parallel processing is required to provide practical computational times for 3D LES of turbulent reacting flows. If detailed, multi-step chemistry is needed, then a significant portion of the calculation will be tied up in the subgrid chemistry modeling. Tabulation and retrieval of reaction rates or integrated reaction increments is needed for efficient use of advanced chemical schemes. An in situ adaptive tabulation (ISAT) method, originally developed by Pope (1997), can be used to represent compositions that are accessed during a given simulation and thus does not require storage for unneeded compositions. Since chemical species evolve through composition space along low-dimensional manifolds, table values are needed for only a fraction of the allowed composition space.

The objective of this study is to evaluate the LES/LEM model for predicting the chemical behavior in lean premixed combustion. An advanced 5-step mechanism, that was derived by steady-state species assumptions from the full GRI2.11 mechanism, was tested. The use of ISAT to store and retrieve reaction rates was also included. LES predictions are compared to laser-based measurements in a bluff-body combustor operating at a lean premixed methane-air equivalence ratio of 0.59.

MODEL DESCRIPTION

The general conservation equations for mass, momentum, energy, and chemical species are filtered to obtain equations for the large-scale (energy containing) variables needed for LES. The filtered equations contain unknown terms such as a subgrid turbulent stress tensor and a

subgrid reaction rate that must be modeled. Unlike typical steady-state turbulence models, the subgrid models for LES are a function of the local grid (or filter) size.

The subgrid turbulence was approximated with the Localized Dynamic Kinetic energy Model (LDKM - Kim and Menon, 1997). Within the LDKM, the eddy viscosity is computed as a function of the local grid size ($\bar{\Delta}$) and the subgrid turbulent kinetic energy (k_{sgs}): $\nu_T = C_r \bar{\Delta} k_{sgs}^{1/2}$. A transport equation for the k_{sgs} is solved and requires terms that are obtained from velocity gradients at a test filter level. The test filter width is taken to be ~2 times the grid filter width. The LDKM has no adjustable constants and is widely applicable to a large range of turbulent flow conditions. Recent studies by McDaniel et al (2002) show good comparisons of experimental data and LES predictions with the LDKM for a lid driven cavity.

The subgrid chemistry was described with the Linear Eddy Mixing (LEM) model (Kerstein, 1992). The LEM utilizes a 1-Dimensional description of the scalar field at lengths down to the molecular level. Molecular diffusion and chemical reaction are treated exactly and turbulent convection within the LES grid is modeled. The influence of turbulent convection is modeled in a stochastic manner by making random rearrangements of the scalar field along the 1D domain. Each event involves the spatial redistribution of the species field within a specified segment of the linear domain. The frequency parameter (λ) and size distribution ($f(l)$) of the segments for rearrangement are obtained from Kolmogorov cascade laws for a high Reynolds turbulent flow according to (McMurtry et al., 1992; 1993):

$$f(l) = \frac{5}{3} \frac{l^{-8/3}}{\eta^{-5/3} - L^{-5/3}}$$

$$\lambda = \frac{54}{5} \frac{\nu Re_L}{L^3} \left(\frac{L}{\eta} \right)^{5/3}$$

where Re_L is the Reynolds number based on the integral length scale, ν is the kinematic viscosity, η is the Kolmogorov scale, and L is the integral scale.

The amount of large scale transport of linear eddy segments between LES grid cells is based on the flux across each cell boundary, as computed from the resolvable grid scale velocity. The LEM segment transport from LES cell to LES cell is called splicing. The splicing events occur at a frequency comparable to the LES time step, which is greater than the time step governing the convection-diffusion-reaction process in the subgrid. Further details on the LEM model and its implementation in a finite-volume CFD code can be found in Zuo et al. (2003).

Two chemical mechanisms were included in the LES modeling reported here. The first mechanism was a simple 1-step methane oxidation mechanism that had been tuned to match laminar flame speeds over a range of equivalence ratio and inlet temperature. The second mechanism was a more advanced 5-step mechanism that had been derived from the 276-step, 49 species, GRI-Mech 2.11 mechanism (Bowman et al., 1996). Steady-state assumptions were applied to 38 intermediate species. The 5-step mechanism consists of four combustion steps and one NO-forming step:

The reaction rates corresponding to this reduced mechanism were obtained from a computer-assisted reduction mechanism (CARM) code developed by Chen (1997) and subsequently reported in Mallampalli et al. (1998). The rate of NO formation was a function of elementary rates in the thermal, prompt, and N_2O - intermediate pathways, and so all three NO - formation mechanisms were represented. The 5-step mechanism has been shown to provide good agreement with the full GRI mechanism for temperature, CO, and NO at lean conditions.

The In Situ Adaptive Tabulation (ISAT) method (Pope, 1997) was used to efficiently store and retrieve 5-step reaction rates that were needed for the LEM. The ISAT method utilizes a binary tree data structure to store reaction information at compositions that are accessed during the LES calculation. Fast retrievals are used for revisited compositions. The ISAT method allowed each node in the binary tree to grow based on the local ellipsoid of accuracy (EOA). The EOA was computed from a Singular Value Decomposition (SVD) and allowed linear extrapolation within a compositional node. An error tolerance of $1\text{E-}5$ was utilized and a maximum of 10,000 entries in each binary tree was allowed. A total of 10 trees, each with a distinct temperature range, were utilized. Once this maximum limit was achieved, the tree was emptied. We have found that the retrieval can be faster if the binary tree is not allowed to grow too large. Overall, a retrieval rate of $\sim 85\%$ was obtained for the LES cases reported here.

Radiative heat transfer was included for some LES cases. The Discrete Ordinates Method (DOM) was used to solve the radiative transfer equation. Local gas absorptivities were computed based on the mass fractions of H_2O and CO_2 .

The LES methodology has been implemented in the unstructured CFD-ACE+ code. The code features a co-located, fully implicit and strongly conservative finite-volume formulation, pressure-based solution algorithm (SIMPLEC), second-order Crank-Nicholson temporal differencing, and second-order central spatial differencing. The CFD-ACE+ flow solver has been parallelized for distributed and SMP architectures using the MPI message passing library and domain decomposition. A parallel cluster of 8 and 15 Linux-based PC's were used for the 2D and 3D LES computations respectively. Each PC includes a 1400 Mhz AMD Athlon chip, 1 Gbyte of DDR-PC2100 RAM and 100-Base-T networking. A parallel scale-up efficiency of 80% has been achieved on this Linux cluster for LES cases distributed on 64 processors (McDaniel et al., 2002). The 1-step LES/LEM cases required ~ 0.17 and 9 hours to achieve 150 timesteps for the 2D and 3D cases, respectively. The 2D, 5-step LES/LEM case, required 3 hours for 150 timesteps. Typically, 2,000-3,000 timesteps were required for accumulating mean-flow statistics.

EXPERIMENTAL SETUP AND BOUNDARY CONDITIONS

Recent experimental data in a bluff-body-stabilized combustor at lean premixed conditions were obtained by Nandula, Pitz, and coworkers (Pan et al., 1991; Nandula et al., 1996). These laser-Doppler anemometry (LDA) measurements of velocity and a combination of Rayleigh scattering, spontaneous Raman scattering, and laser-induced fluorescence (LIF) measurements were obtained to provide a source of information with which to evaluate combustion models. The uncertainty involved in the species and temperature measurements, based on a single-shot uncertainty analysis, is given in Table 1.

Table 1. Uncertainty in Chemical Species Measurements and Temperature Measurements from Nandula et al (1996)

Scaler	% Error
CH ₄	3.3
O ₂	7.5
H ₂ O	5.1
CO ₂	5.1
NO	7.6
CO	17.6
Temperature	1.0

The combustion chamber, shown in Figure 1, was configured such that a stainless steel conical bluff body of base diameter 44.45 mm and apex angle 45° was mounted coaxially at the center of the combustor and served as a flame holder. The burner enclosure consisted of a square cross-section with filled round corners.

Figure 1. Schematic and Turbulent Flame Structure of Bluff-Body-Stabilized Lean Premixed Combustor (Nandula et al., 1996)

The LES model was run with an axisymmetric geometry (8892 cells) and a full 3D geometry (1015488 cells) as shown in Figure 2. The mass-flow rate for the combustor was specified by using the measured values reported for the air (3960 slpm) and the CH₄ fuel (244 slpm). This corresponded to a CH₄-air equivalence ratio of 0.59. A turbulence grid was placed at the entrance of the combustor section, upstream of the bluff-body. The free stream turbulence at this inlet was measured to be 24% (based on a 15 m/s mean velocity). Appropriately scaled turbulence levels were set in the LES model at the inlet for the boundary condition of k_{sgs} . An inlet temperature of 300 K and a combustor pressure of 1 atm were also specified in the model. Wall temperatures for the combustor and bluff-body were set to 500 K. For cases with radiation, the wall emissivities were set to 0.2.

Figure 2. Structured Grids for 2D-axisymmetric Approximation and Actual 3D Combustor Geometry

2D vs. 3D LES MODEL RESULTS

LES modeling was performed for the small 2D-axisymmetric cases and the full 3D case. The cross-sectional area of the 2D case was equal to the actual 3D cross-section. Due to the high computational expense of the 3D case, only 1-step chemistry with LEM was utilized. Time steps of 7.5E-6 seconds were used and were small enough to resolve the eddy turnover times of the smallest energy containing scales. The 3D case was decomposed onto 15 processors and still required ~800 Mbytes of RAM for each processor during the LES run. This high memory usage was primarily due to the LEM that stores scalar information within each LEM subgrid element. This high memory requirement needs to be improved for clusters with smaller amounts of RAM and so that multi-step chemistry can be realized.

Instantaneous snapshots of temperature for the 2D axisymmetric case and the 3D case are shown in Figure 3. The axi-symmetric results show less large-scale mixing than the 3D results. The 3D results shows the penetration of unburned reactants all the way to the combustor centerline. This

mixing pattern indicates that there is a non-symmetric vortex that occurs about the combustor centerline. Figure 4 shows instantaneous temperature and k_{sgs} contours at $x/d = 0.71$. These non-symmetric mixing patterns will play a role in predicting the correct level of emissions and temperature in the combustor. The 3D LES calculations are still being performed in order to obtain enough samples for time-averaged statistics.

Figure 3. Instantaneous Temperature Contours Along Combustor Axis for 2D Axisymmetric and 3D Cases

Figure 4. Instantaneous $x/d = 0.71$ Contours of Temperature and k_{sgs} at 0.009 and 0.01125 seconds

A monitor point was placed one inch downstream of the bluff-body dump plane in the shear layer. Figure 5 shows the time history of pressure at this location for the 2D case. Also shown is the fourier transformed signal from the 2D analysis. A strong frequency near 222 Hz was predicted. This frequency is close to the natural $\frac{1}{4}$ wave frequency for the ambient temperature combustor geometry. The small structures observed in the 2D snapshot seem to correspond to a higher frequency of ~ 800 Hz. This 800 Hz frequency is detected in the temperature signal, but is not so strong in the pressure signal shown here.

Figure 5. Predicted Pressure History in Bluff-body Shear Layer for 2D Axisymmetric Case

TEMPERATURE AND MAJOR SPECIES

Comparisons of measured and predicted time-averaged temperature and major species were performed at various axial locations in the combustor. 2D LES modeling with the LEM subgrid chemistry was utilized with either 1-step and 5-step mechanisms. Also, the effect of radiative heat transfer on the predictions was evaluated.

Figure 6 shows time-averaged temperature predictions for the 1-step and 5-step mechanisms. The steady-state RANS results approach a non-reacting solution. The non-reacting RANS solution could not be avoided, even when the inlet equivalence ratio was initially much higher than the actual value and slowly reduced. The results show small differences in the flameshape near the flameholder for the two chemical mechanisms. This indicates that the 1-step and 5-step mechanisms capture overall similar heat release rates. The 1-step LEM results show a slightly faster overall reaction rate since the flame is wider and less unburned fluid exits the combustor. Figure 7 shows comparisons between time-averaged temperature predictions and measurements at several axial locations. Overall, the results are in good agreement with the experimental data for the LES/LEM cases. The results show the strong need for using LES/LEM in order to sufficiently mix the products and reactants and stabilize the flame. The SS RANS case was not able to resolve the enhanced reaction rates due to turbulent mixing. The LEM calculations were performed with radiative heat transfer. The radiative heat transfer reduced near bluff-body product temperatures by ~ 100 K compared to adiabatic.

Comparisons of the measured and predicted rms temperature profiles are shown in Figure 8. Overall the agreement with the data is reasonable at this $x/d=0.1$ location. The models slightly underpredict the temperature fluctuations in the recirculation zone behind the bluff-body. The LES/LEM models captured the radial location of peak temperature fluctuation. The 5-step mechanism results produced lower fluctuations in the shear layer than the 1-step model. Unfortunately, measured rms values at other downstream locations were not available from the experiment to further evaluate the models.

Figure 8. Comparison of Measured and Predicted rms Temperature at $x/d=0.1$

Comparisons of measured and predicted major species are shown in Figures 9 through 12. Many of the same conclusions from the temperature comparisons can be made for the major species. The CH_4 mole fractions are well predicted in the hot product zone behind the flameholder. At $x/d = 1.0$, the 5-step mechanism gives better agreement in the shear layer, as it predicts a nearly fully burned flame at r/d values near 0.4. At $x/d = 6.0$, the 1-step mechanism actually gives a better prediction as more of the flow exits the combustor as burned products.

Figure 9. Comparisons of Predicted and Measured Time-Averaged CH_4 Mole Fraction Profiles

Figure 10. Comparisons of Predicted and Measured Time-Averaged O₂ Mole Fraction Profiles

Figure 11. Comparisons of Predicted and Measured Time-Averaged CO₂ Mole Fraction Profiles

Figure 12. Comparisons of Predicted and Measured Time-Averaged H₂O Mole Fraction Profiles

The mean O₂ mole fraction comparisons indicate a very slight overprediction in the hot product zone just downstream of the bluff-body for both chemical models. The agreement is well within the measurement error for the O₂ measurements at most locations. As observed earlier, the 2D LES/LEM results are not able to fully capture the full mixing that produces a nearly uniform flow of hot products at the final axial location ($x/d=6$) near the combustor exit.

The CO₂ and H₂O mole fraction comparisons are again quite good. There is an overprediction of H₂O concentrations at the nearest location to the bluff-body ($x/d=0.1$). This may indicate that intermediate radicals have not fully converted to water in the actual experiment. The model predicts nearly complete conversion of the radicals to CO₂ and H₂O along the centerline behind the bluff-body.

MINOR SPECIES

The measured fields of CO, NO, and OH were compared with the predictions from the 5-step LES/LEM model. Predictions with radiation and without radiation are shown. Figures 13 through 15 show the minor species comparisons at the various axial locations. It is clear that the 2D axisymmetric LES/LEM model with 5-step chemistry does only a fair job at matching the measured concentrations of minor species. As observed in the CO results, the radial location of peak concentration is captured, but the magnitude is overpredicted by 2-3 times for x/d locations less than 0.6. At $x/d = 1.0$, the comparisons are relatively good in the reacting shear layer. At $x/d = 6.0$, the CO concentrations are overpredicted towards the outer wall and underpredicted near the centerline. This discrepancy is probably due to the overall underpredicted mixing from the 2D axisymmetric model.

Figure 13. Comparisons of Predicted and Measured Time-Averaged CO Mole Fraction (ppm) Profiles

Figure 14. Comparisons of Time-Averaged NO Mole Fraction (ppm) Profiles

Figure 15. Comparisons of Time-Averaged OH Mole Fraction (ppm) Profiles

The comparisons in Figure 14 show that the NO levels are underpredicted by as much as 6 ppm. This is a relatively large discrepancy given the low 8-12 ppm levels that were measured in this combustor. The experimenters do caution that the reported NO levels could be 2-3 ppm higher than actual levels due to unaccounted for interference of O₂ on the NO laser measurements. It is not clear how the NO predictions could be improved. Comparisons with the full GRI mechanism show 5-step NO predictions to actually be 1-2 ppm higher than the full mechanism. It could be possible that the underpredicted mixing in the 2D model prevents the correct formation and destruction of intermediate radicals that contribute to the enhancement of prompt and N₂O mechanisms for this lean premixed system. The contribution of the thermal pathway is small for this case due to the low lean premixed combustion temperatures (~1600 K). The negligible contribution of the thermal pathway can be deduced from the radiation and adiabatic cases that gave ~100 K different combustion temperatures but nearly no change in NO emissions.

Comparisons of OH mole fractions are shown in Figure 16. The predicted OH concentrations are higher than the measured levels at nearly all combustor locations. Only at $x/d = 1.0$ are the comparisons reasonable. The adiabatic equilibrium OH levels are ~200 ppm and the 5-step LES model predicts super-equilibrium levels that are as high as 2000 ppm. It is not clear if the 3D modeling with stronger mixing will lower the OH levels. The OH levels predicted by the 5-step and the full GRI mechanism should be compared for single point Perfectly Stirred Reactor (PSR) calculations to see if discrepancies in the reduced mechanism exist.

CONCLUSIONS

Laser-based measurements from a methane-air, bluff-body-stabilized, lean premixed combustor were used to evaluate the LES/LEM model. A comparison of the predictions and measurements showed that the mean temperature and major species were captured reasonably well with the 2D axisymmetric LES/LEM model. Without LEM, reaction rates were not sufficiently enhanced to even hold a stable flame. Comparisons of measured and predicted (5-step LES/LEM) minor species such as CO, NO, and OH were not as good as the major species. It seems that full 3D modeling with multi-step chemistry will be needed to capture the non-symmetric turbulent structures and may provide better agreement with the minor species.

3D LES modeling with LEM will be needed in the robust and efficient design of combustion systems. Full 3D LES/LEM modeling is expensive, both in terms of CPU time and RAM, even for 1-step chemical mechanisms. The 3D results shown here indicate that significantly different turbulent structures are captured compared to 2D results. The use of chemical tables that include subgrid turbulent stirring will be needed to eliminate the memory and cpu time limitations in 3D. Work involved with the training of artificial neural nets (ANNs) in a stand-alone LEM code over a range of subgrid turbulence and chemical compositions is underway. Once sufficiently trained, these turbulent ANNs would be used in the full 3D LES calculation and would replace the expensive on-line LEM completely.

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APPENDIX D — GEORGIA TECH DOE-HAT COMBUSTOR LES