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

First Year Program Review

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ABSTRACT

In this project, an advanced computational software tool will be developed for the design of low emission combustion systems required for Vision 21 clean energy plants. This computational tool will utilize Large Eddy Simulation (LES) methods to predict the highly transient nature of turbulent combustion. The time-accurate software will capture large scale transient motion, while the small scale motion will be modeled using advanced subgrid turbulence and chemistry closures. This three-year project is composed of: Year 1 - model development/implementation, Year 2 - software alpha validation, and Year 3 - technology transfer of software to industry including beta testing. In this first year of the project, subgrid models for turbulence and combustion are being developed through university research (Suresh Menon-Georgia Tech and J.-Y. Chen- UC Berkeley) and implemented into a leading combustion CFD code, CFD-ACE+. The commercially available CFD-ACE+ software utilizes unstructured, parallel architecture and 2nd-order spatial and temporal numerics. To date, the localized dynamic turbulence model and reduced chemistry models (up to 19 species) for natural gas, propane, hydrogen, syngas, and methanol have been incorporated. The Linear Eddy Model (LEM) for subgrid combustion-turbulence interaction has been developed and implementation into CFD-ACE+ has started. Ways of reducing run-time for complex stiff reactions is being studied, including the use of in situ tabulation and neural nets. Initial validation cases have been performed. CFDRC has also completed the integration of a 64 PC cluster to get highly scalable computing power needed to perform the LES calculations (~ 2 million cells) in several days.

During the second year, further testing and validation of the LES software will be performed. Researchers at DOE-NETL are working with CFDRC to provide well-characterized high-pressure test data for model validation purposes. To insure practical, usable software is developed, a consortium of gas turbine and industrial burner manufacturers has been established to guide and direct the software development/validation effort. The consortium members include Siemens-Westinghouse, GE Power Systems, Pratt & Whitney, Rolls-Royce, Honeywell, Solar, Coen, McDermott, Vapor Power, Woodward FST, Parker Hannifin, John Zink, RamGen Power, Virginia Tech, DOE-NETL, Air Force Research Laboratory, DOE-ANL, and NASA GRC. Annual consortium meetings are being held in Huntsville, with the 2nd meeting scheduled for January 31-February 1, 2002.

Benefits of the program will include the ability to assess complex combustion challenges such as combustion instability, lean blowout, flashback, emissions and the effect of fuel type on performance. The software will greatly reduce development costs and the time cycle of combustor development. And perhaps the greatest benefit will be that the software will stimulate new, creative ideas to solve the combustion challenges of the Vision 21 plant.

INTRODUCTION

Vision 21 combustion systems will require innovative low emission designs and low development costs if Vision 21 goals are to be realized. In the past, relatively few combustion designs could be studied and experimentally tested due to the excessive expense of combustion testing. Using today's design/analysis tools, many innovative designs needed for the Vision 21 plant will remain on the drawing board, and only incremental improvements may be realized. What is needed, is a new, reliable analysis tool for the design of combustion systems that will significantly reduce development costs. With such a tool, new combustor designs can be easily studied, and only the best designs selected for experimental testing. The effect of fuel type on performance can easily be assessed. This software tool should reduce the time-cycle from inception to production, permitting development of new combustion systems in time to meet Vision 21 time table goals.

OBJECTIVE

The overall objective of this project is to develop and validate a Large Eddy Simulation (LES) computational tool that can be used in the efficient design of low emission combustion systems for Vision 21 clean energy plants. The combustion LES software will include state-of-the-art subgrid turbulence and chemistry models and should be able to accurately simulate the highly transient nature of gaseous-fueled turbulent combustion. Efficient numerical algorithms that rely on in situ look-up tables and artificial neural networks will be utilized in an unstructured, parallel CFD flow solver. The specific objectives of the project are:

1. to develop reduced chemical mechanisms that provide accurate representation of emissions (CO and NO_x), ignition delay, and heat release;
2. to incorporate the LES formalism with advanced subgrid scale turbulence models into a finite-volume turbulent reacting flow solver on arbitrary grids;
3. to implement advanced subgrid chemistry models (LEM and CMC) into the LES code;
4. to optimize the speed of the LES code by using advanced algorithms (such as ISAT and neural networks) and parallelization;
5. to validate the LES code in benchmark configurations, by comparison with existing numerical or experimental data, for model validation and refinement purposes;
6. to apply the resulting software tool to the design of combustion systems relevant to the Vision 21 program with the direct participation of industry partners;
7. to package the LES code as a complete commercial software tool that is user-friendly and robust.

APPROACH

In this project, a 3D, unstructured grid, parallel LES combustor design code will be developed and evaluated for predicting emissions and thermal-acoustic instabilities in advanced gaseous fueled combustion systems. Detailed chemical mechanisms capable of describing emissions, ignition delay and heat release, for various gaseous fuels (natural gas, syngas, hydrogen, and biogas) over a wide range of conditions will be identified. Reduced chemical mechanisms will then be developed (12-20 species) by assuming certain species reach a steady-state with respect to other intermediates, reactants, and products at conditions of interest to the design engineer. Once the chemical mechanism has been reduced, the in situ adaptive tabulation and neural networks will be utilized to efficiently compute, store, and retrieve reaction rate information for the full, 3D LES calculation. The effects of turbulence on the chemical kinetics will be described with the linear eddy model (LEM). The LEM includes an exact description of molecular diffusion and reaction in one dimension at the laminar viscosity scale and requires a model for turbulent convection. The goal of the project is to develop an LES code that contains the state-of-the-art in turbulent combustion modeling on a parallel platform that can be user friendly as well as practical for combustor design. A team of qualified personnel from university research institutes (Suresh Menon at Georgia Tech; J.-Y. Chen at UC Berkeley) and CFDRC has been assembled to develop and then implement the necessary submodels into the commercial LES code. The LES code will then be evaluated with lab-scale experimental data and applied to predicting emissions and thermo-acoustic instabilities for advanced configurations supplied by gas turbine combustor and industrial burner manufacturers with direct involvement and participation.

The project has been divided into 12 tasks and to cover a 3-year time frame. The first year is focused primarily on model development, the second year on model optimization and testing, and the third year on beta testing of the code by industrial consortium members. The specific tasks during the first year are:

Task 1. Develop Reduced Chemical Mechanisms: Reduced chemical mechanisms will be developed from the appropriate full mechanisms for: i. natural gas, ii. syngas, iii. hydrogen, iv. biogas at conditions of interest that provide accurate representation of emissions (CO and NOx), ignition delay and heat release.

Task 2. Develop an In Situ Adaptive Tabulation Module: The In Situ Adaptive Tabulation (ISAT) method will be implemented in a general purpose module. This module will later be used with the LEM/CMC models and with the reduced chemical mechanism to allow for efficient chemical kinetic computations.

Task 3: Implement LES Framework: The LES framework will be implemented into the 3D, unstructured-grid, parallel, flow solver in CFD-ACE+. The code will be modified to include specific LES boundary and initial conditions, and processing of the data (averaging and monitor points routines). To make the final product user-friendly, this task involves the modification of the CFD-GUI to include the setup for the new problem conditions and models.

Task 4: Select and Implement Advanced Subgrid Turbulence Models: The dynamic models for the SGS stresses and scalar fluxes will be implemented into CFD-ACE+. A dynamic subgrid

turbulence model for describing the local turbulent kinetic energy will be implemented in the code. This subgrid turbulence model will provide necessary input for the LEM subgrid chemistry model.

Task 5: Development and Implementation of the LEM Subgrid Chemistry Model: The Linear Eddy Model (LEM) which characterizes the interactions of turbulence and chemistry at the subgrid scale will be developed and implemented into the CFD-ACE+ package. This model will allow the accurate simulation of low emission reacting flows in non-premixed and premixed regimes.

Task 6: Development and Implementation of the CMC Subgrid Chemistry Model: As a less expensive computational alternative, the CMC formulation will be developed and implemented in the LES code to be used for both non-premixed and premixed regimes. The CMC formulation will contain two conditioning variables, mixture fraction/progress variable and the scalar dissipation/progress variable dissipation.

Task 7: Implement Tabulation Schemes for the Reduced Chemical Mechanisms: This task involves interfacing the tabulation modules, In Situ Adaptive Tabulation (ISATPD) and Artificial Neural Networks (ANN), with the LES code. Specifically, the subgrid chemistry models, CMC and LEM, will be coupled with these tabulation routines.

Task 8: Parallelization of LES Code: The MPI protocol will be used to parallelize the new LES features of the CFD-ACE+ flow and chemistry solver and the MDICE code. This extension will allow for testing of the 3D LES capability on unstructured grids with parallel computing and differential physical modeling.

Industrial Consortium

An industrial consortium was organized with following purposes: (1) to guide and direct software development and validation, and (2) to transfer the LES software to industry. The consortium members are shown in Figure 1. Annual consortium meetings are held at CFDRC, with the 2nd meeting planned for January, 2002.

Figure 1. Combustion LES Consortium Members

PROJECT DESCRIPTION

The proposed combustion LES software is the latest CFD methodology for turbulent-reacting flows, providing accuracy and reliability not available from current CFD methods. Current CFD analysis consists of 2D and 3D Reynolds Averaged Navier Stokes (RANS) calculations that use two-equation k-ε models for turbulence, and very simplified chemistry for heat release. The unsteady motions that govern mixing (i.e. countergradient diffusion) cannot be captured by the k-ε turbulence model. Two-step and four-step chemistry (with five or fewer species) is not sufficient to model the minor species that contribute to prompt and nitrous NO_x and CO emissions. With current RANS codes, the effect of turbulence-combustion interaction is approximated by the Eddy Break Up (EBU) or Eddy Dissipation models (Spalding, 1977) which assume the reaction is controlled by either mixing or chemistry, but never a combination of the two. NO_x and CO emissions are very difficult to predict, especially for new designs at sub-10 ppmv levels.

The proposed LES method simulates the large scale turbulence numerically, and uses more-universal models for subgrid turbulence and chemistry. This allows a more accurate representation

of turbulence, kinetics, and turbulence-combustion interaction not attainable with RANS calculations. It also allows more detailed chemistry to be modeled, including the calculation of minor species needed for accurate prediction of NOx and CO, lean blowout, and autoignition/flashback. A snapshot of a typical LES calculation performed by CFDRC for a liquid-fueled, high performance combustor is shown in Figure 2. It can be seen that fine structures in the scalar field are well captured, and the flame looks much different than its steady-state RANS counterpart in Figure 3. LES methods accurately capture the coupling between unsteady heat release and system acoustics, thus predicting combustion dynamics and limit cycle pressure oscillations. A time history comparison of predicted and measured combustor pressures of the high performance combustor is presented in Figure 4, showing good overall agreement.

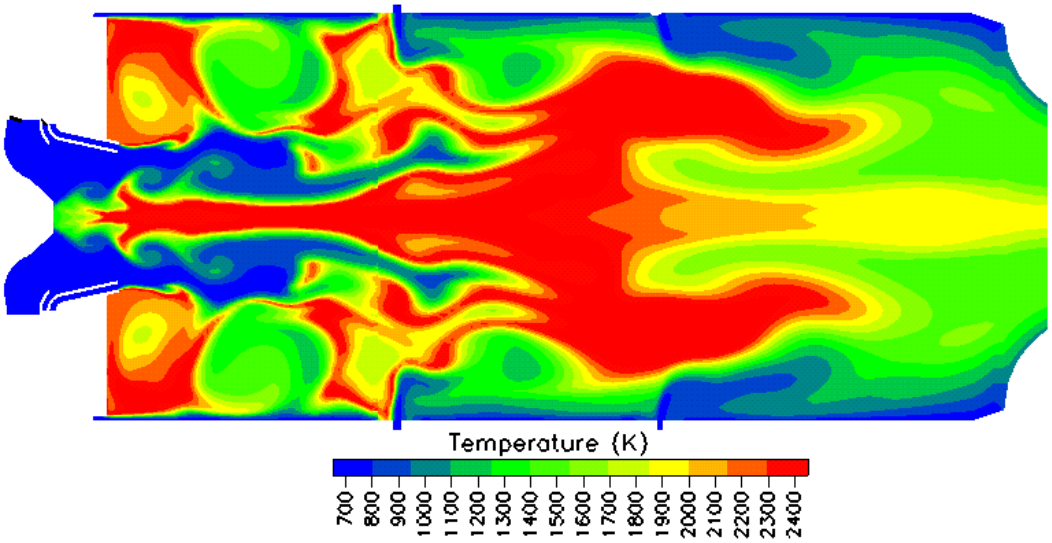

Figure 2. Snapshot of LES Calculation of Liquid-Fueled, High Performance Combustor, Temperature Distribution

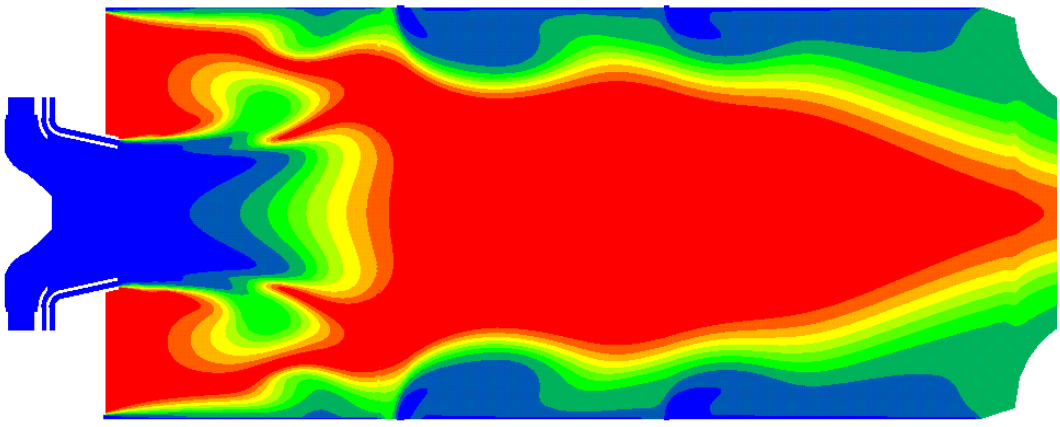

Figure 3. RANS Calculation of Liquid-Fueled, High Performance Combustor, Temperature Distribution

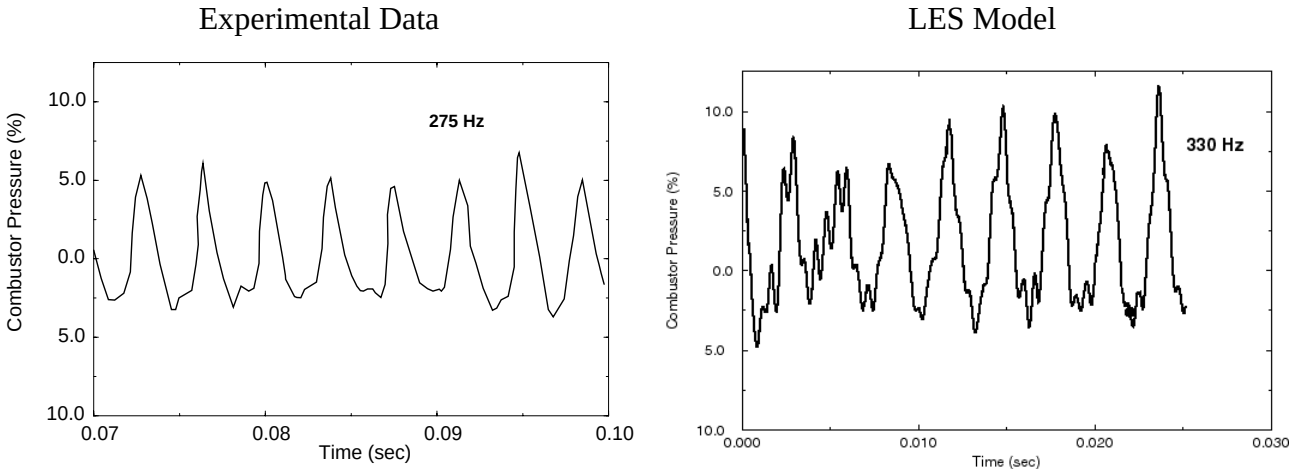

Figure 4. Good Engineering Agreement between Measured and Predicted Limit Cycle Pressures

Starting LES Code

The starting point in the development of the LES code is an existing Navier-Stokes solver integrated in a commercial CFD software package, CFD-ACE+ (CFD Research Corporation, 1999). CFD-ACE+ is the culmination of expertise obtained from 14 years of CFD development and commercialization at CFDRC. CFD-ACE+ is a fluids, heat and mass transfer simulation system based upon a parallel implementation of an unstructured flow solver. This system is comprised of four modules:

- CFD-GEOM: A geometry modeler, mesh generator
- CFD-GUI: A graphical user interface for pre-processing the solver
- CFD-ACEU: A parallel, pressure-based, polyhedral unstructured solver
- CFD-VIEW: A visualization package/post-processing tool.

These application modules are all integrated via the CFD-DTF common file format and library. This publicly available common file format/library enables many important features in the unstructured flow solver, allowing the treatment of multiple-domained grids containing structured, unstructured and polyhedral-unstructured meshes in a fully implicit manner, as if they were consolidated into a single "virtual" zone.

CFD-ACEU is a finite-volume, pressure-based, unstructured flow solver. It supports conservation volumes comprised of arbitrary polyhedra, including the more commonly used types, such as hexahedra, tetrahedra, prisms, quadrilaterals and triangles. It uses a fully implicit procedure based upon the SIMPLE/PISO algorithm, and employs first-, second- and third-order spatial discretizations, as well as first- and second-order temporal schemes

FIRST YEAR RESULTS

Reduced Chemistry

Several reduced chemical mechanisms have been developed for methane, propane, and hydrogen combustion by Prof. J.-Y. Chen of UC Berkeley. Detailed reaction mechanisms were used as the starting point and included: GRI2.11 and 3.0 (Bowman et al., 1996) for methane and hydrogen; Miller NO_x reactions (Barlow et al., 2001); and Koert et al., (1996) for propane. An interactive computer-assisted reduction mechanism code (CARM) was utilized to automatically generate the reduced chemistry. CARM uses the following procedures.

(a) A detailed mechanism is used to solve a PSR for certain combustion conditions. The solutions contain information on species concentrations, rates of production, and species sensitivity coefficients.

(b) Quasi-steady-state (QSS) species are selected based on their concentration levels as well as on the rate-of-production analysis.

(c) After selection of the QSS species, a set of independent elementary reaction steps is chosen to eliminate the QSS species in order to permit systematic construction of the reduced mechanism, using the matrix operations proposed by Chen (1988). The subroutine that computes the chemical source terms is automatically generated once the reduced mechanism is constructed.

This subroutine is compatible with CHEMKIN and returns the molar production rates of the species given the pressure, temperature, and mass fractions. A coupled set of nonlinear QSS species equations are numerically solved within the subroutine to provide the necessary elementary reaction rates for the reduced mechanism. For example, calculations were performed for the partially premixed Tsuji flames measured by Barlow et al (2001) and comparisons with the data were made. Figures 5a and 5b compare measurements with predictions using the reduced and detailed chemistry. These results show excellent agreement between the reduced and detailed mechanisms.

The methane, propane, and hydrogen mechanisms have all given excellent results compared to the full mechanism. For syngas combustion, the methane mechanism should be appropriate, since syngas is comprised mainly of CO and H_2, and these submechanisms are included in GRI2.11.

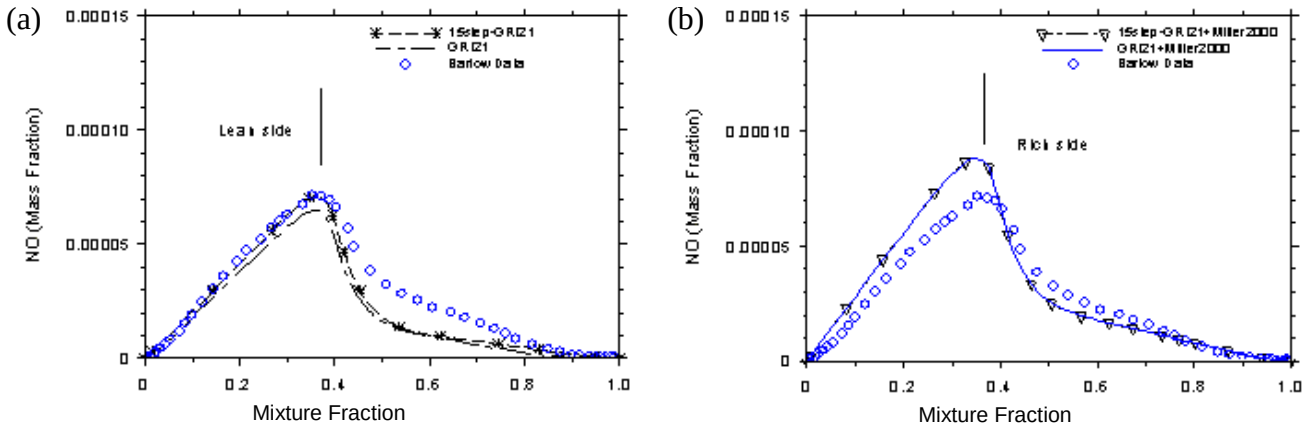

Figure 5. Comparison of Measured and Predicted NO Using (a) GRI2.11+Miller and (b) GRI2.11 + Miller Detailed Mechanisms with 15-step Reduced Chemical Mechanisms.

Reduced Mechanism Implementation in CFD-ACE+ (DOE NETL Unstable Combustor)

The capability of predicting instability using the reduced chemical kinetic mechanisms was demonstrated. A 19 species methane mechanism was developed from a combined full mechanism for natural gas combustion. The full chemistry consisted of the GRI2.11 mechanism and a newly developed mechanism from Miller for NO. The combined mechanism more accurately describes NO emissions at rich conditions compared to the stand-alone GRI mechanism.

The 19 species reduced mechanism consists of the following 15 global steps:

(1) H + HO2 = H2 + O2
(2) H + H2O2 = H2 + HO2
(3) 2OH = H2 + O2
(4) OH + CH3 = H2 + CH2O
(5) H + CH4 = H2 + CH3
(6) H + OH + CO = H2 + CO2
(7) 2H = H2
(8) CH2O = H2 + CO
(9) H + O2 + HCN = H2 + CO + NO
(10) O2 + C2H2 = H2 + 2CO
(11) OH + C2H4 = H2 + CH3 + CO
(12) C2H6 = H2 + C2H4
(13) H + OH = H2O
(14) H + CO + N2 = NO + HCN
(15) 2H2 + OH + NO = 2H + O2 + NH3

Thirty-one species are assumed to be at steady-state, so their full transport equation is not needed. But, their concentrations must be computed from the tracked (non-steady-state species) in order to compute the elementary rates. This inner iteration requires more computational time than standard Arrhenius mechanisms, but the accuracy is typically better. Also, the reduction in the number of species from 50 to 19 is significant in terms of memory requirements for the LES code and for chemical look-up tables. The computations that are reported here were done with direct integration.

The chemistry was handled with operator splitting, where a stiff ODE solver was used to accurately represent the simultaneous set of chemical kinetic equations.

Unsteady RANS calculations were performed for the 2D axisymmetric DOE combustor geometry (Richards and Janus, 1997). The 2D grid was decomposed into 13 domains and parallel computations were performed in parallel on CFDRC's cluster of Linux-based PC's. Figure 6a shows the predicted unstable limit cycle of pressure inside the combustor. A 6.5% pressure oscillation is observed. The Discrete Fourier Transfer (DFT) of the signal is shown in Figure 6b and clearly indicates a strong oscillation at 258 Hz. Table 1 shows the oscillation results for the experiments compared to predictions using 1-step mechanism and the 15-step reduced mechanism.

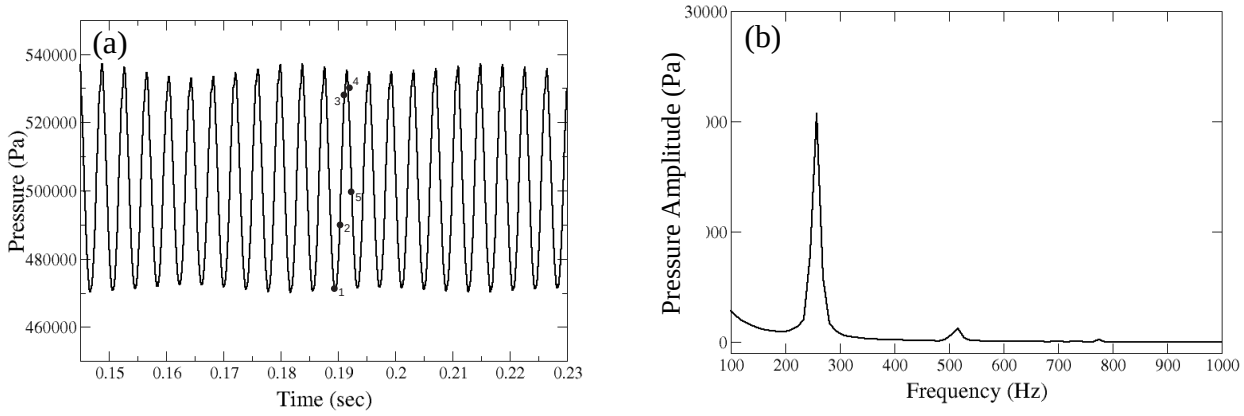

Figure 6. (a) Predicted Combustor Pressure History and (b) Corresponding Spectrum Using 19 Species Chemistry

Table 1. Predicted and Measured Oscillations in the Unstable DOE-NETL Case

	Magnitude	Frequency
Measured	6.4%	225 Hz
15-Step Chemistry	6.5%	257 Hz
1-Step Chemistry	6.8%	256 Hz

These results show that the chemistry does not have a strong effect on the predicted oscillation. This is likely due to the strong driving mechanism of a convective time-lag from the fuel injection location to the flame zone. The chemical times are certainly much smaller than the convective transport times and therefore have a very small effect on the predicted instability. The more detailed chemistry will provide superior results if strong extinction/ignition effects are present and if accurate emissions are needed. These results do show that the 15-step reduced chemistry is implemented correctly in the LES code and that successful convergence can be obtained for this unstable combustion case.

Instantaneous snapshots of pollutant emissions can be observed during the instability cycle. The predicted CO mass fraction during the oscillation cycle is shown in Figure 7.

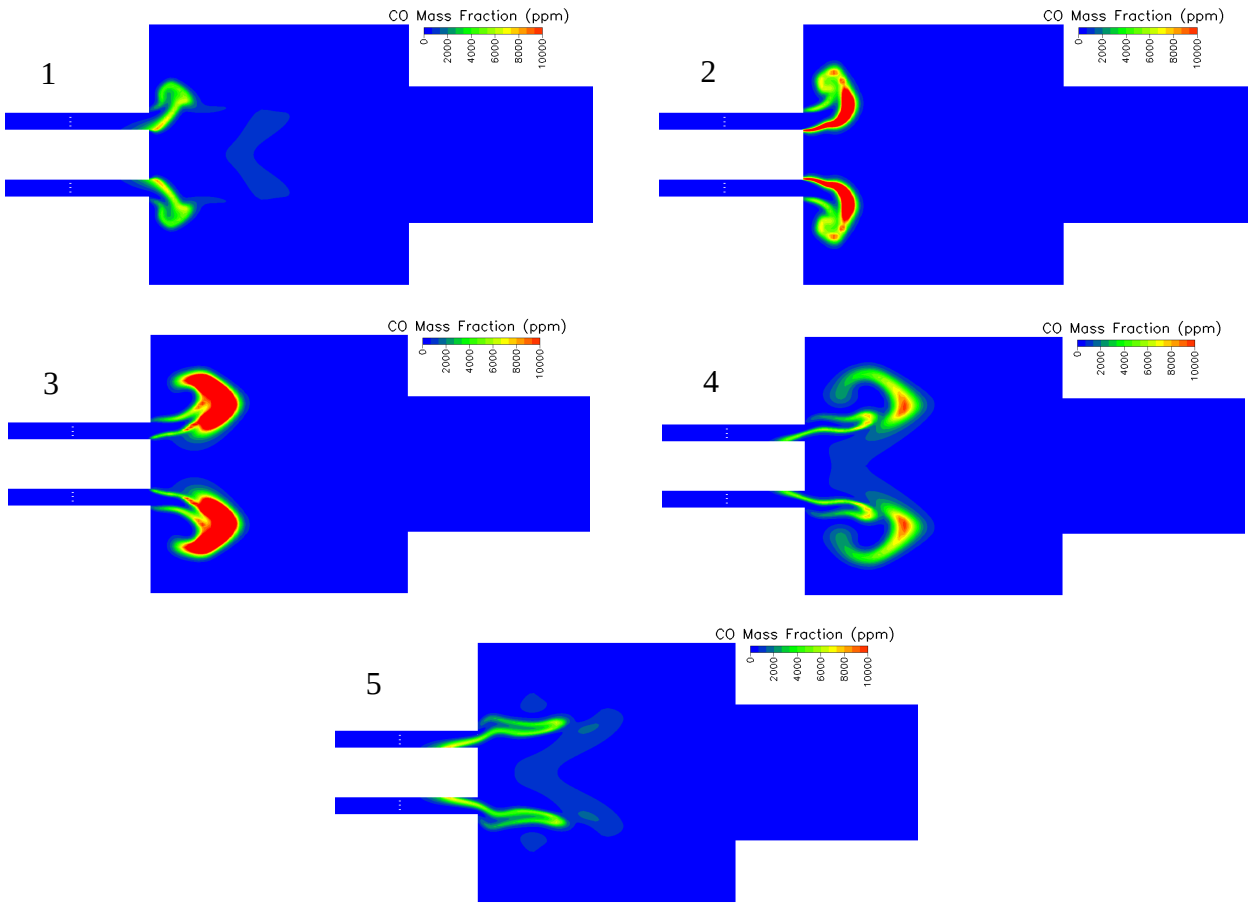

Figure 7. Predicted CO Mass Fractions During the Unstable Cycle [Unsteady RANS with 19 Species Chemistry]

The CO mass fraction contours show significant regions of high CO during the high pressure portion of the cycle. At the low pressure portion of the cycle, the CO regions are collapsed towards the centerline and are much smaller. It is known that maximum heat release occurs when CO and other intermediates are oxidized. It is very likely that maximum heat release would occur between points 3 and 4 in the cycle when the peak CO at time 3 oxidizes to significantly lower values at time 4. It is also interesting to observe a separated region of high CO at point 4 in the cycle. This separation occurs due to the high shearing that occurs during the oscillation. The unstable flow shows a strong flapping motion in the axial and radial directions.

In addition to the 19 species reduced mechanism, a skeletal mechanism containing 84 elementary reactions from the GRI mechanism was also tested in the LES code. This mechanism does not require the expensive inner iteration on steady-state species, but does require the solution of 21 species equations and is not as accurate as the 19 species reduced mechanism. It was found that computational times were twice as fast as the 19-species mechanism calculations. Despite this improvement in speed, the computational time was still too slow since it would take ~ 40 days for a

full 3D case. The ability to replace direct integration with table look-up must be accomplished in order to produce practical run times.

In Situ Adaptive Tabulation (ISAT)/Pk-Tree Data Structure

The original ISAT algorithm (Pope, 1997), for generating on-the-fly look-up tables of chemical reaction rates, was implemented in CFD-ACE+. ISAT was tested for the 19-species mechanism on several cases including the unstable DOE combustor. Initial results indicated that ISAT could work for small 2D cases that remained relatively stable. But, for large amplitude combustion instability cases the table size continued to grow even after the available RAM (768 MD per processor) was used up. Figure 8 shows a comparison of combustor pressure in the DOE-NETL case using ISAT versus direct integration for the 19-species chemistry. Good accuracy can be obtained with ISAT, but 80-90% of the chemical kinetic calculations were still additions (direct integration) rather than retrievals. The table fills up after ~ 2000 timesteps. Figure 9 shows results with less error control. As shown, poor results are obtained if the table is not allowed to grow.

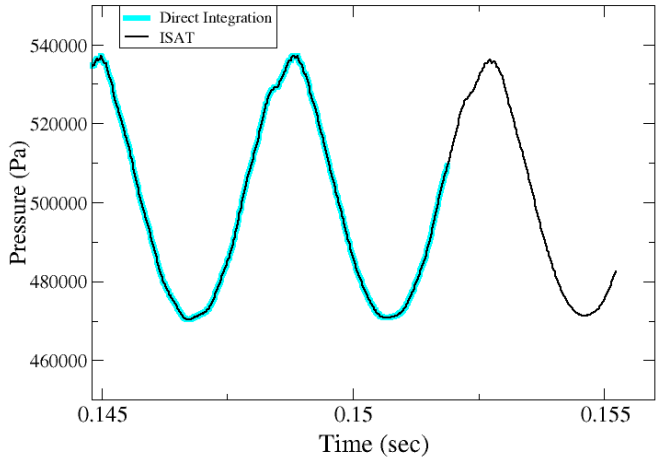

Figure 8. Comparison of ISAT (high error control) with Direct Integration for Unstable DOE Combustor

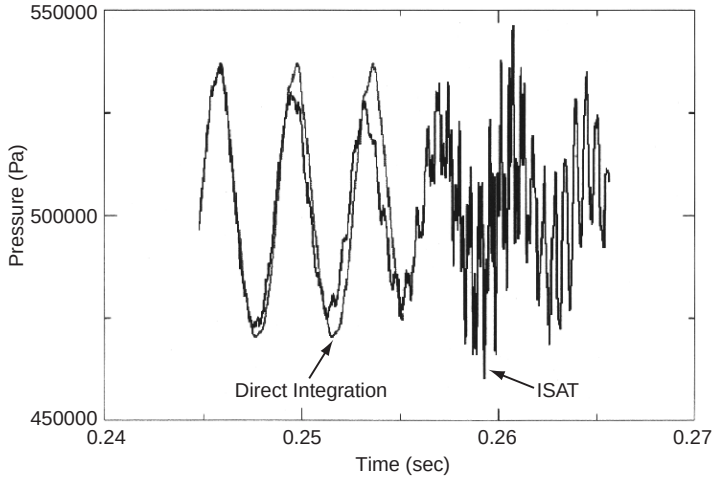

Figure 9. Comparison of ISAT (low error control) with Direct Integration for Unstable DOE Combustor

These original ISAT results indicate a previously observed problem in the binary tree data structure. That is, difficulties in locating nearest neighbor compositions and thus a duplication of records. Professor Menon at Georgia Tech has eluded to this potential problem in his recent work (Kapoor et al, 2001). Specifically, the following shortcomings with the original ISAT were identified:

a. the binary tree structure (BSP-tree) can become highly unbalanced, leading to inefficient storage and expensive searches;
b. for a given composition query the search algorithm does not guarantee the return of the nearest neighbor, thus leading to unnecessary duplication of the stored data; and
c. when the method was extended to reuse a generated ISAT table, it was found that even when starting from the same initial conditions, the algorithm added new records in the binary tree.

Based on a review of existing data structures and multi-dimensional access methods, a Pyramid K-instantiable (PK) tree was investigated and is being implemented in ISAT.

The PK-tree is described in detail by Yang et al (1997). This tree structure differs from all existing trees by using a unique set of constraints to eliminate unnecessary nodes that can result from a skewed spatial distribution of objects. This ensures that the total number of nodes in a PK-tree is O(N) and the average height is of O (log N). A remarkable set of properties of PK-trees include: non-overlapping of sibling nodes and uniqueness of the tree for a given set of data points. Computational studies have shown that the PK-tree outperforms other methods. The preliminary evaluations have shown that PK-tree can reduce storage requirements up to 50% compared to the current indexing method used in the ISAT module and allows for very efficient nearest-neighbor searches. The code is in a development/testing stage and should be fully operational in CFD-ACE+ during the upcoming year.

Localized Dynamic (LDKM) Subgrid Turbulence Model

The localized dynamic (subgrid-scale) kinetic energy model (LDKM) developed originally by Kim and Menon (1997) was implemented and tested in the LES combustion code. The LDKM model used scale-similarity and the subgrid-scale kinetic energy $k_{sgs} = \frac{1}{2}\left(\overline{u_k u_k} - \overline{u_k}\,\overline{u_k}\right)$ to model the unresolved scales. With this model, a test filter is required to locally computer adjustable coefficients that are needed to close the subgrid scale kinetic energy transport equation. With arbitrary grids, the test filter consists of a weighted average of the cells sharing a node with the current cell. The LDKM is relatively simple and efficient and is applicable to various flowfields without adjustment of the model. The LDKM has been tested for a back-step flow and a lid driven cavity. (a)

Back-Step Test Case: The LDKM has been initially validated in simulations of isothermal shear layers formed at the rearward facing step. LES results were compared with experimental data taken from Pitz and Daily (1983). The experimental configuration consists of a rectilinear section followed by a smooth contraction to one half of its height, a step expansion into the test section, and a converging exit region. The tests were conducted at atmospheric pressure and the mean velocity and temperature at the inlet are 13.3 m/s and 293 K. These conditions give a Reynolds number of 22,100 using the step height as the characteristic length. The computational grid

consisted of 376,256 cells decomposed into 15 domains. Cells were clustered near the shear layer and towards the wall. Wall functions were used for RNG k-ε steady-state calculations and Van Driest Damping was utilized for the near-wall, Smagorinsky LES calculations. A fixed velocity and pressure were imposed at the inlet and outlet boundaries, respectively. Random fluctuations were imposed on the velocity at the inlet. Periodicity was assumed at the streamwise boundaries. Second order differencing in space (Central) and time (Crank-Nicholson) were utilized. The transient simulations were performed with a time step of 1.6e-5 seconds (maximum Courant number of 0.22) for a total of 0.504 seconds (~12 flow through times). Statistics were collected after the initial perturbation had settled out at approximately 5 flow through times. Mean and rms velocity profiles were obtained and compared to experimental data.

The inlet 13.3 m/s flow forms a shear layer downstream of the dump. Velocity and pressure oscillations occur in this shear layer. Figure 10 shows a snapshot of axial velocity at 0.496 seconds. The formed structures are irregular and 3-dimensional in nature.

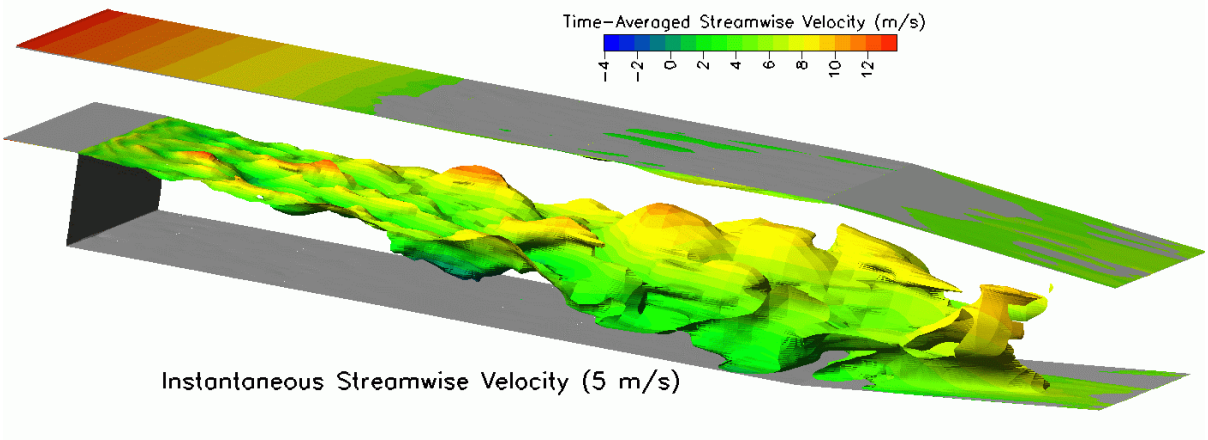

Figure 10. Predicted Instantaneous Streamwise Velocity (5 m/s) at 0.496 Seconds Using LDKM

The measured length of the recirculation zone extends 7 step heights from the dump. The LDKM predicts a reattachment length of 6.91, the Smagorinsky predicts 6.84, and the unsteady RANS (RNG k-ε) predicts 6.93. What is most interesting is that unsteady RANS does not predict any unsteady motion (i.e., unsteady RANS produces a steady-state solution), yet there is little difference between LES and unsteady RANS results for this nonreacting backstep case. Figure 11 shows comparisons between measured and predicted axial velocity profiles at various X/H locations. These results show reasonable agreement with all three models for the mean velocity profiles. All three models underpredict the spreading rate of the shear layer. At the furthest downstream location, separation occurs at the top wall using the Smagorinsky model. The RNG k-ε and LDKM models do a better job of predicting the flow at this downstream, top wall region.

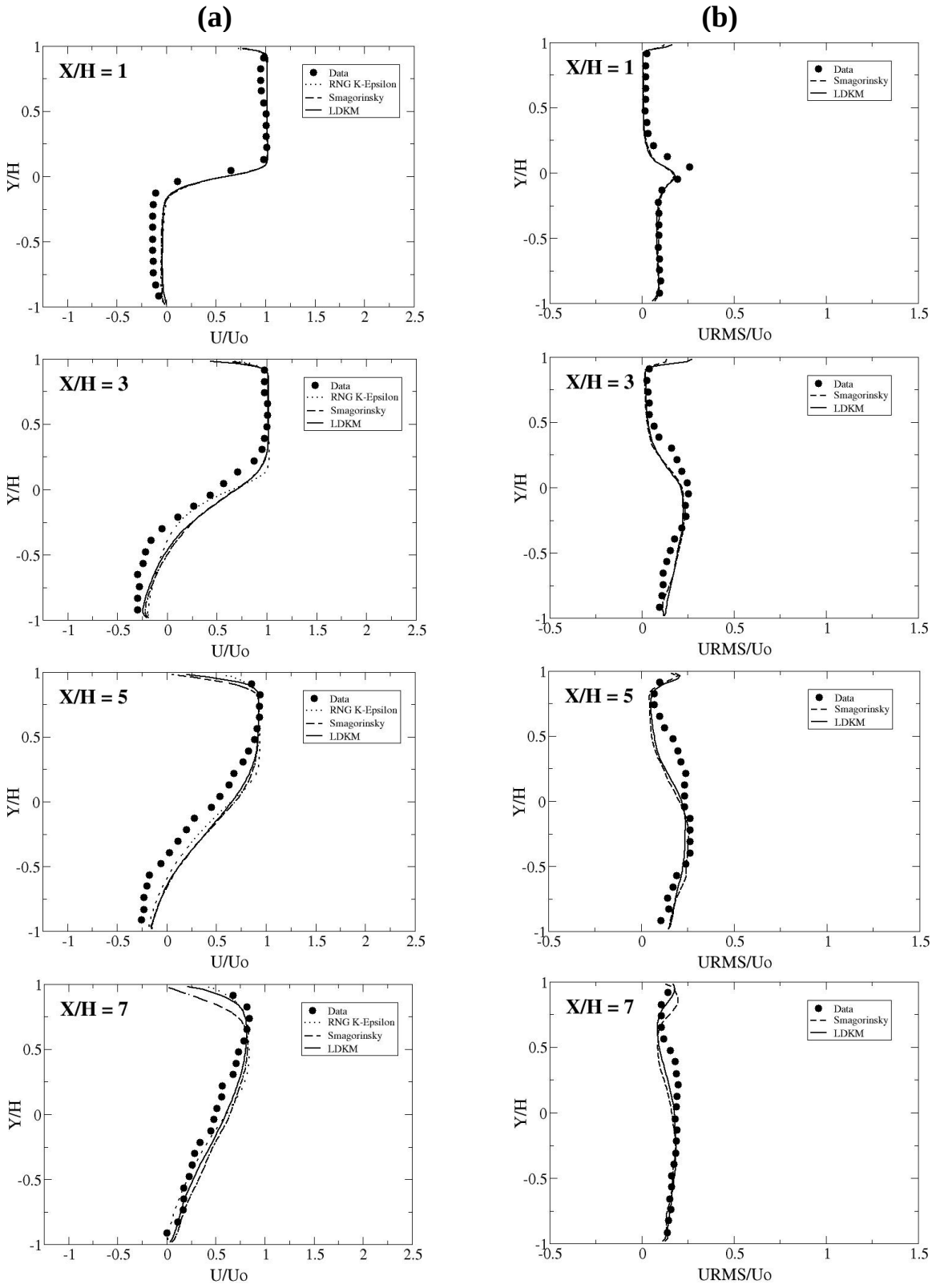

Figure 11. Comparison of Time-averaged Velocity Profiles of Streamwise (a) mean and (b) rms Velocity at Various Axial Locations

Despite the similar mean flow field predictions between the RNG k-ε and full LES, the LES simulations will be needed to predict more complex situations that occur in swirling and reacting flows. Swirling turbulent flows introduce less isotropy and more non-equilibrium turbulence than the present back-step case. Also, the LES-predicted unsteady motions are important in capturing flame shapes and emissions that must be determined for robust combustor design.

Lid Driven Cavity

Measured data from a lid-driven cavity experiment (Prasad et al., 1998) was also used to validate the LDKM subgrid turbulence model in the LES code. Three-dimensional cavity flows are highly non-homogeneous with complicated flow patterns; consisting of a primary vortex and several corner vortices. The resolution of the computational grid was 64x64x32 (123039 cells). The grid was uniform in the Z direction and stretched towards the walls in the X and Y directions. The flow conditions were specified as:

U_b = .06 m/s
T = 298.15 K
ρ = 997 Kg/m^3
Cp = 4184 J/Kg-K

Isothermal boundary conditions were used for all the walls including the lid. The U_b was imposed on the top wall to simulate the moving wall in the experiment. The RNG k-ε turbulence model was used for the unsteady RANS calculation and the LDKM with dynamic coefficients was used for the subgrid closure in the LES calculation. Figure 12 shows the normalized mean U-velocity along the Y-centerline.

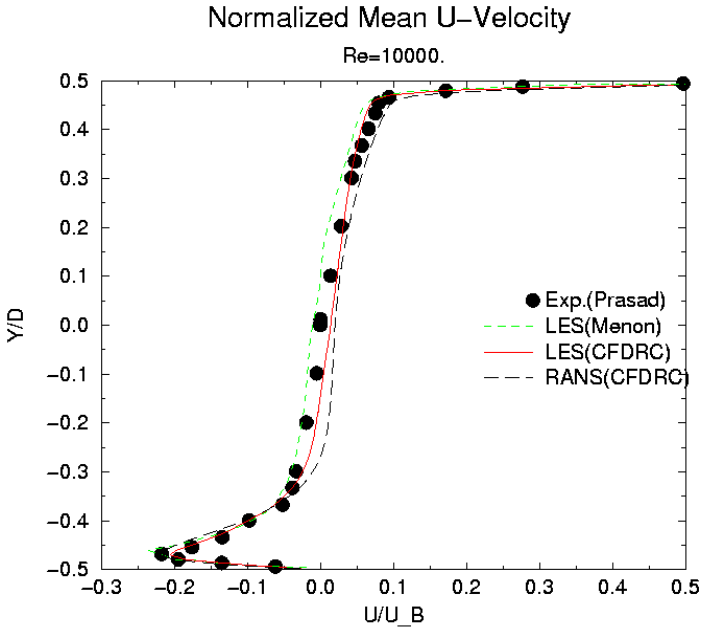

Figure 12. Normalized Mean U-Velocity

Both the LES and RANS calculations capture the mean velocity at the lower boundary wall. The LES predicts the mean velocity in the core flow and along the top wall better than the RANS calculation. This LES calculation is consistent with the LES calculation performed by Kim and Menon (1997). The Normalized U-RMS is shown in Figure 13.

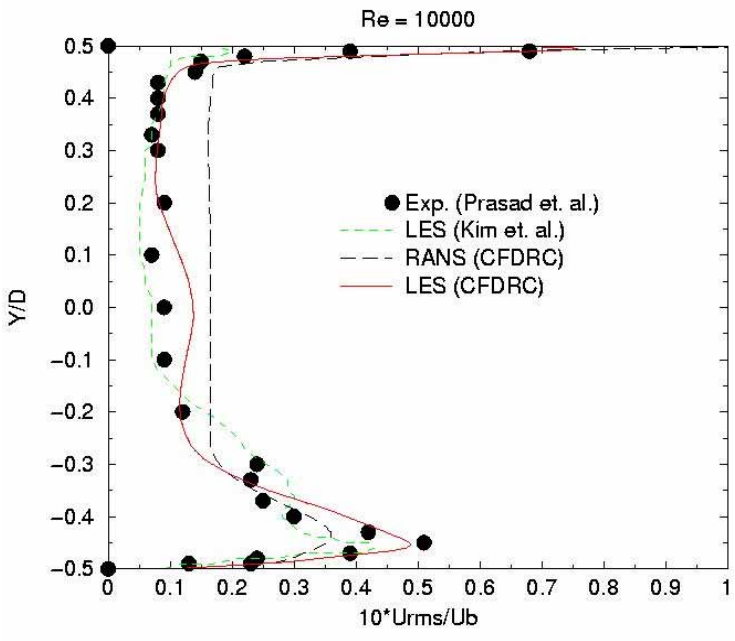

Figure 13. Normalized U-RMS Along Y-Centerline in Midplane

The LES simulations by CFDRC better predicts the U-RMS at the bottom wall compared to the LES by Kim and Menon (1997), and the RANS simulation by CFDRC. It also compares better to data near the lid than that of Kim. The U-RMS near the center peaks at .15 for the LES-CFDRC simulation. The unsteady RANS underpredicts the peak RMS at the bottom wall and overpredicts the RMS in the core flow. Overall, these results show that the LDKM is working correctly in the LES code and provides better results than unsteady RANS.

Linear Eddy Model (LEM) with Artificial Neural Nets (ANN) for Subgrid Chemistry

The LEM subgrid chemistry model and ANN approach (for faster LEM) are being developed by Georgia Tech. The LEM (developed by Kerstein (1988)) is well suited as a subgrid chemistry model for LES since it provides an exact description of chemical kinetics and molecular diffusion at all length scales of the flow, while modeling the effects of turbulent advection. This is achieved by formulating the model in one spatial dimension. Turbulent advection is simulated by making random rearrangement events and using an appropriate PDF for the size distribution of eddies.

For engineering applications, only simple 1-step chemistry can be used with an on-line LEM implementation. With multi-step chemistry, a look-up table approach will be needed to replace expensive chemical kinetic integrations. For large mechanisms (> 15 species) a neural net approach may be required since the table size can become too large. Initial validation of the ANN approach, by Georgia Tech, was carried out for a single cell Linear Eddy reaction zone. The ANN was trained at certain turbulent conditions in the thin reaction zone regime and was then used to

accurately predict combustion at non-trained turbulent conditions. Figure 14 shows the instantaneous and time-average profiles of the major species and temperature using direct integration/ISAT and ANN. As shown, the ANN is capable of capturing the behavior of a new flame. These results were performed for 5 species (1-step) chemistry and are now being extended to 8 and 19 species mechanisms. The ANN will also be extended to include the subgrid kinetic energy and grid filter width as independent variables.

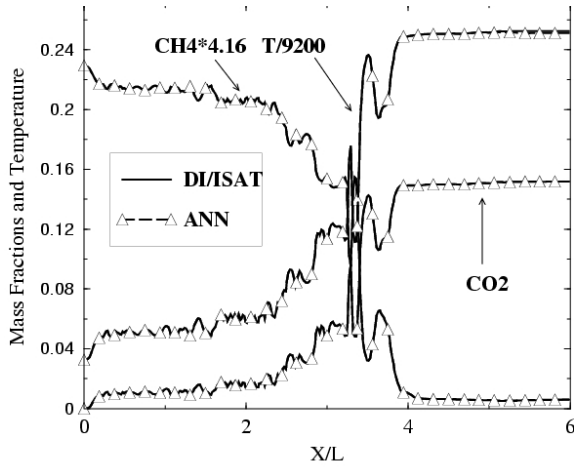

Figure 14. Instantaneous Flame F2 Profiles Predicted by Combining 2 ANNs (for F1 and F3). Results compared to direct integration by ISAT.

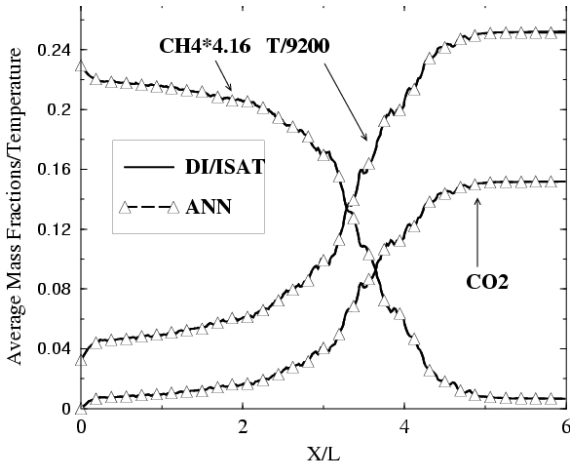

Figure 14. Time-average Flame F2 Profiles Predicted by Combining 2 ANNs (for F1 and F3). Results compared to direct integration by ISAT.

Parallel Performance of LES Cluster

The parallel performance of the LES code has been improved during this first year. The Linux based cluster of 64 PC's are connected through a 100 BASE-TX Ethernet Fully Connected Network Topology. The four switches are connected to a 3Com matrix module creating one virtual switch between all 64 processors. Load balancing of the communication domain, data buffering, and synchronization are parallel issues that have been found to affect the performance of the LES software applied on the Linux cluster.

Load balancing of the communication domain must be considered when using a large number of processors. Large synchronization times can develop if the number of neighboring processors differs for a given processor. For example, a processor with 3 neighbors will have to wait on a processor with 6 neighbors. The k-way partitioning implemented in Metis (domain decomposition software use in CFD-ACE+) minimizes the amount of transfer data but doesn't balance the number of neighboring processors. This is difficult to accomplish in a graph decomposition, but can be achieved through geometrical decompositioning. If a partitioning along an orientation axis can be achieved, then the number of neighbors for each domain will be load balanced (excluding end domains). The significant improvement in parallel performance for an x-cut decomposition versus an arbitrary (k-way) decomposition was shown for the backstep case.

The packing of ghost cell data was improved by storing a map of the ghost cell position. This increases the required memory slightly but decreases the extent of the packing loop. The loop now

goes over the surface of ghost cells rather than over the total volume of cells. This has a greater effect for domains with a small surface to volume ratio.

Typical LES runs require 5-10 sweeps on the pressure correction equation for each iteration. Also, a timestep will require 5-10 iterations to obtain convergence. Previous parallel calculations transferred data at each sweep within the solver for each variable to maintain an implicit solution for the entire flowfield. A zonal implicit method was then implemented (for the CGS solver) so that data transfer only occurred at the end of each iteration. This new approach slightly decreases the solver accuracy, but for transient calculations with small timesteps (as needed for LES), the convergence can be maintained with no more than double the number of iterations per timestep.

These parallel improvements were applied to a transient simulation of a three-dimensional incompressible lid driven cavity. In order to assess parallel performance the number of timesteps, iterations, and sweeps were held constant for all runs to maintain a constant computational load. A structured grid with dimensions 191x191x95 was used. Figure 15 shows the speedup of compute time on the LES cluster. The speedup obtained for the 64 processor case was 52 which is about an 80% efficiency. The efficiency of the original parallel method (fully implicit) in CFD-ACE+ was only 60% for the same 64 processor case. These significant improvements in the parallel speedup are important for performing practical engineering LES.

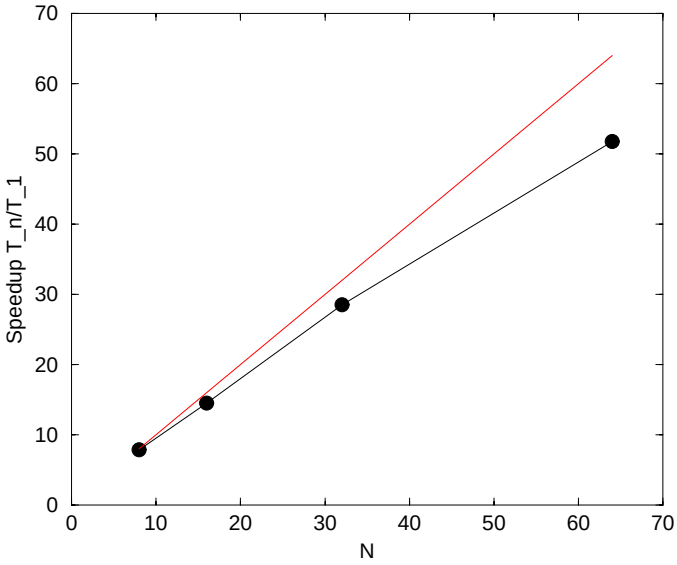

Figure 15. Speedup vs. Number of Processors

Selection of Test Cases

Test cases for evaluating the LES combustion code were examined. The new experimental data from the DOE-NETL swirl combustor (Maloney, 2001) will be one of the test cases since it will include a comprehensive data set (velocity, species, temperature, dynamic pressure) over a large range of conditions, including high pressure. DOE-NETL has developed these experiments with well defined acoustic boundary conditions that will be needed for evaluating the code. Another data set of interest will be the lean premixed, swirling combustion data of Gore et al (2001). This Purdue data was acquired through a DOE-ATS contract for validating gas turbine combustion CFD

codes. They cover a range of flow rates including stable and unstable combustion. They also capture instantaneous images of flame structure throughout the unstable combustor cycle. These images will be valuable validation of the LES capability for predicting instability. GE and Fluent are currently using the Purdue DOE data for evaluating their combustion codes.

The low pressure data of Pitz and coworkers at Vanderbilt (Nandula et al., 1998) will be used to validate the emissions capability of LES. They have detailed NO and CO measurements at sub 10 ppm levels. This bluff-body lean premixed data will provide a strong test of the code.

These cases will be presented in detail at the consortium meeting in January 2002. Other possible cases may be considered, depending on feedback from the participants.

APPLICATION

The combustion LES code, once tested and validated, will be an important tool in the design of advanced gaseous combustion systems. The software will be able to model the transient nature of turbulent combustion and allow assessment of complex combustion challenges including: combustion instability, lean blowout, flashback, emissions, and effect of fuel type. The LES code will allow the combustion engineer greater insight into the combustion process and will help stimulate new ideas. This design tool should reduce combustor development costs and the time cycle of combustor development.

FUTURE ACTIVITIES

Work during the upcoming, second year will include further development and implementation of subgrid models and alpha testing of the LES code. Several selected cases will be analyzed from both a hydrodynamical and chemical performance point of view. Comparisons between numerical and experimental results for the selected test cases will be performed. During Year 3, the code will be applied to industrial design concepts related to Vision 21 energy plants. Charter members of the industrial consortium will provide beta testing of the code. Based on comments and results from this beta testing, needed improvements will be incorporated into the LES code. Improvements will include user friendliness issues (modifications to GUI) as well as accuracy issues (modifications to physical models).

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