LES SOFTWARE FOR THE DESIGN OF LOW EMISSION COMBUSTION SYSTEMS

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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. Vision 21 combustion systems, such as combustors for gas turbines, indirect fired cycles, furnaces, and sequestrian-ready systems, will require innovative low emission designs and low development costs if Vision 21 goals are to be realized. The proposed simulation tool will greatly reduce the number of experimental tests, will stimulate new ideas, will provide the capability of assessing and adapting low-emission combustors to alternate fuels, and greatly reduce the development time cycle of combustion systems.

This revolutionary computational tool will utilize Large Eddy Simulation (LES) methods to accurately simulate the highly transient nature of turbulent combustion. The time-accurate LES software will numerically capture large-scale transient motion, while the small-scale motion will be modeled using advanced subgrid turbulence, chemistry, and turbulence-combustion interaction closures. In this way, combustion LES simulations can predict many combustion phenomena that, until now, were impossible to predict with state-of-the-art 3D steady-state Reynolds Averaged Navier-Stokes (RANS) analysis. With combustion LES software, it will be possible to calculate combustion dynamics (coupling of unsteady heat release and acoustics), pollutant emissions, lean blowout, flashback, autoignition, etc. LES methods are becoming more and more practical by linking together tens to hundreds of PCs and performing parallel computations with fine grids (millions of cells). Such simulations, performed in a few days or less, provide a very cost-effective complement to experimental testing. In five years, these same calculations can be performed in eight hours or less due to the expected increase of computing power.

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 were developed by expert university researchers (Dr. Suresh Menon of Georgia Tech and Dr. J.Y. Chen of University of California, Berkeley), and are being implemented into a leading combustion CFD

code, CFD-ACE+. The commercially available CFD-ACE+ software utilizes unstructured, parallel architecture and accurate 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 JP8 have been incorporated into CFD-ACE+. The Linear Eddy Model (LEM) for combustion-turbulence interaction has been developed and implemented into CFD-ACE+. 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.

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 Solar, GE Power Systems, Pratt & Whitney, Rolls Royce, Honeywell, Coen, McDermott, Vapor Power, Woodward FST, Parker Hannifin, John Zink, RamGen Power, Siemens-Westinghouse, Virginia Tech, DOE-NETL, Air Force Research Laboratory, DOE-ANL, and NASA GRC. Seven consortium members will perform beta testing of the software on their advanced combustion systems. In this way, the software will penetrate the industrial market and be used in the design environment. An initial consortium meeting was held in November 2000, and a second meeting occurred in January 2002. A third meeting will occur in November 2002 to transfer the code and train users.

CFDRC has also completed the integration of a 64 PC computer cluster to get highly scalable computing power needed to perform the LES calculations in days, rather than weeks. This effort has developed super-computing capabilities at a fraction of the cost of a large computer of equal power.

Another key ingredient of this project is code validation against data from realistic geometry at realistic test conditions. Researchers at NETL's Gas Energy Systems Dynamics Division are working closely with CFDRC to provide well-characterized high-pressure test data for model validation purposes. Historically, validation of complex computer models has been a problem, but this weakness is being addressed in this project. An experiment has been designed with government and industry cooperation, and testing will be performed at NETL's high-pressure combustion facilities. Sandia National Laboratory is also involved and will provide advanced diagnostic capabilities as well as low-pressure validation data.

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. 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 compressible turbulent reacting flow solver on arbitrary grids;
3. to implement advanced subgrid chemistry models (LEM) 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.

INDUSTRIAL CONSORTIUM

An industrial consortium was organized with the 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. Two consortium meetings have been held at CFDRC, with the 3rd meeting planned for November, 2002.

Industrial Consortium

Charter Members

1. Rolls Royce-Allison
   M.S. Anand
2. Honeywell
   Jurgen Schumacher
3. Solar Turbines
   Mel Noble / Alan Kubasco
4. Coen
   Paul Matys
5. McDermott Technologies
   Alan Sayre
6. Parker Hannifin
   Erlendur Steinthorsson
7. Pratt & Whitney
   Jeff Lovett
8. GE Power Systems
   Shiva Srinivasan
9. Woodward FST
   George Kalinovich
10. Vapor Power
    Thanh Tran

Non-Charter Members

1. Virginia Tech
   Uri Vandsburger
2. Siemens-Westinghouse
   Rich Valdes
3. RamGen Power
   Jon Tonouchi
4. John Zink
   Carol Schnepper

Government Members

1. DOE-NETL
   Dan Maloney
   Tom O'Brien
   David Huckaby
2. Air Force
   Balu Sekar
3. DOE-ANL
   Tom Obot
4. NASA GRC
   Nan-Suey Liu

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.

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, compressible, 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 through 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, hydrogen, and syngas 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. 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 the GRI mechanism.

Reduced Mechanism Implementation in CFD-ACE+

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.

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. Table 1 shows the oscillation results for the experiments compared to predictions using the 15-step reduced mechanism. Overall good agreement was obtained.

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

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 2.

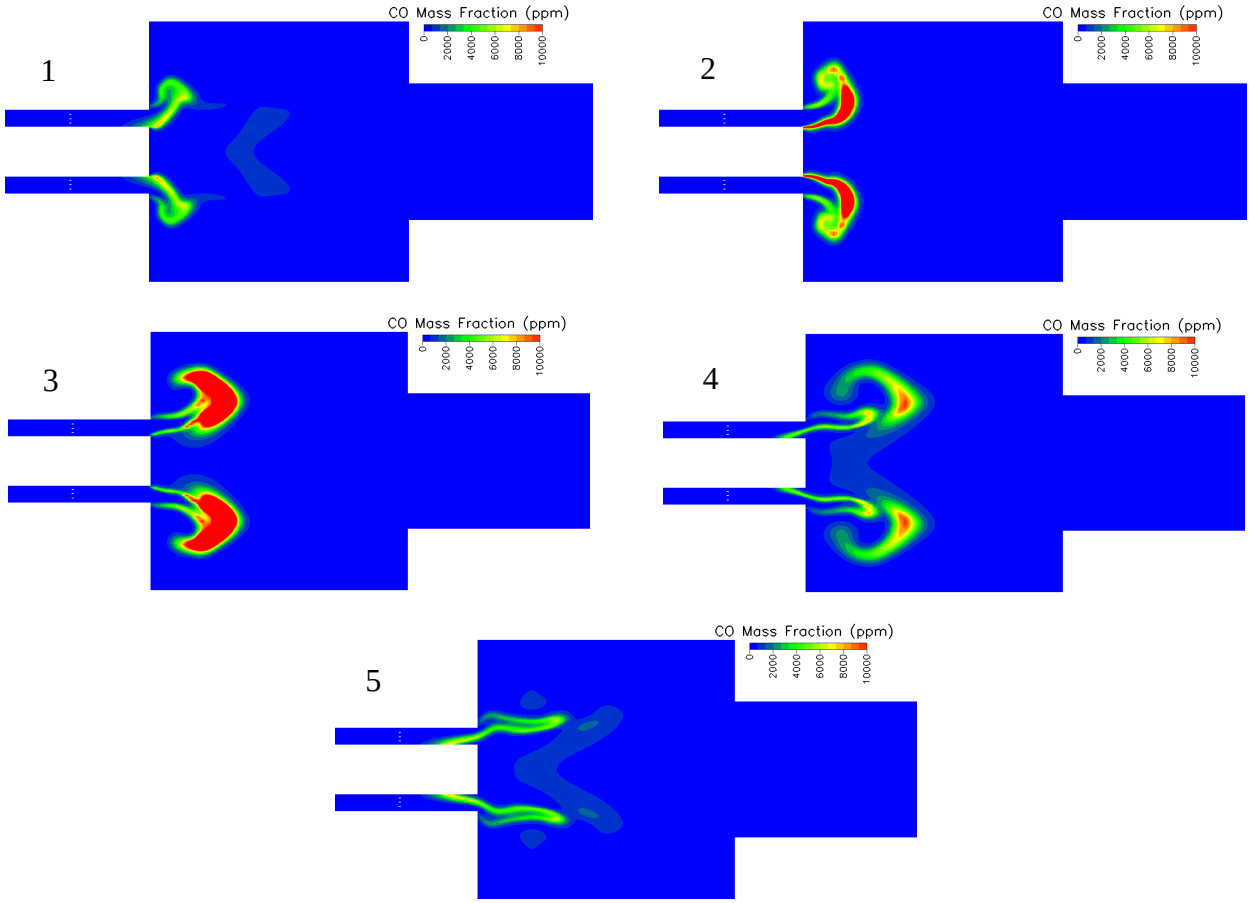


Figure 2. Predicted CO Mass Fractions During the Unstable Cycle [Unsteady RANS with 19 Species Chemistry]

In Situ Adaptive Tabulation (ISAT)

The ISAT algorithm (Pope, 1997), for generating on-the-fly look-up tables of reaction rates, was implemented in CFD-ACE+. ISAT was tested for the methane 5-step (9 species) and 15-step (19 species) reduced mechanisms. The DOE-NETL SimVal Case (Maloney, 2002) was used to test the ISAT method. The lean premixed combustor condition includes a perfectly premixed choked inlet at an equivalence ratio of 0.5, T_{in} of 533 K, and a pressure of 5.1 atm. A 2D axisymmetric geometry was assumed. ISAT results for the various mechanisms are presented in Table 2. A speed-up of ~4 was achieved with the use of ISAT and the 5-step mechanism. Further speed-up is achieved by computing reaction rates only once per time-step (staggered chemistry approach).

Figure 3 shows predicted transient pressure results with ISAT and direct integration. Good agreement was found for the 4x faster ISAT method. Overall, ~80% of the kinetics computations were retrievals for this ISAT case. A tighter tolerance (~73% retrievals) was needed to predict OH and NO concentrations in the central recirculation zone. Comparisons of major species, temperature, and velocity were excellent between direct integration and ISAT for either tolerance level.

Table 2. Direct Integration (DI) and ISAT Results for Transient Combustor CFD Calculations

Premixed Case Mechanism	Kinetics Solution	Error Tolerance	% Retrieves	CPU Time
5-step	DI/Non-Staggered	—	—	400 min.
5-step	DI/Staggered	—	—	39 min.
5-step	ISAT/Non-Staggered	1e-4	88	91 min.
5-step	ISAT/ Staggered	1e-4	82	17 min.
5-step	ISAT/ Staggered	1e-4 (tighter radicals)	73	22 min.
15-step	DI/Staggered	—	—	45 min.
15-step	ISAT/ Staggered	1e-4	35	66 min.

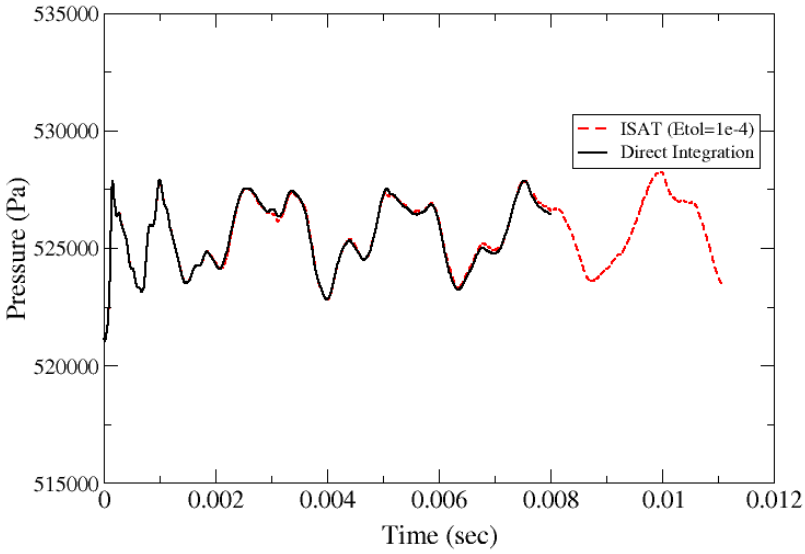


Figure 3. Comparison of Combustor Pressure History Using Direct Integration and *ISAT for the 5-step, 9-species Chemistry*

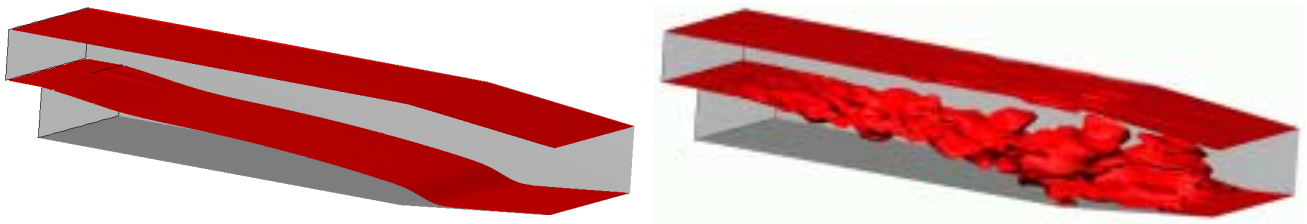
For the 15-step chemistry, a speed-up was not achieved with ISAT, even though 35% of the computations were retrievals. The results showed that for more detailed chemistry, the retrieval process was fairly expensive - even more than direct integration. Pope and coworkers have reported speedups of 10-100 for Monte Carlo PDF calculations. To achieve this speed-up, ~99% of the chemical kinetic calculations would need to be fast retrievals. Approaches for improving the ISAT method are being investigated, including: multiple tree storage, more accurate mapping gradient solution, more accurate and/or efficient singular value decomposition, and a more efficient tree structure (PK-tree). These new improvements in ISAT will be needed to do efficient LES calculations with the 15-step mechanism.

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 compute 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.

Back-Step Test Case: The LDKM has been initially validated in simulations of isothermal shear layers formed at a backstep. LES and unsteady RANS 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. 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 flow forms a shear layer downstream of the dump. Velocity and pressure oscillations develops in this shear layer. Figure 4 shows a snapshot of axial velocity predicted with unsteady RANS and LES (LDKM). Irregular and 3-D structures are formed using LES. Unsteady RANS does not vary much from the steady RANS solution. Despite the significant differences with the instantaneous fluctuations, the mean flowfield predictions were similar.



Unsteady RANS LES

Figure 4. Predicted Instantaneous Streamwise Velocity (5 m/s) using Unsteady RANS and LES

Lid Driven Cavity Test Case: 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
Re = 10,000

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 5 shows the normalized mean and RANS U-velocity along the Y-centerline.

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 LES simulations by CFDRC better predicts the U-RMS at the bottom wall compared to the other models. 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.

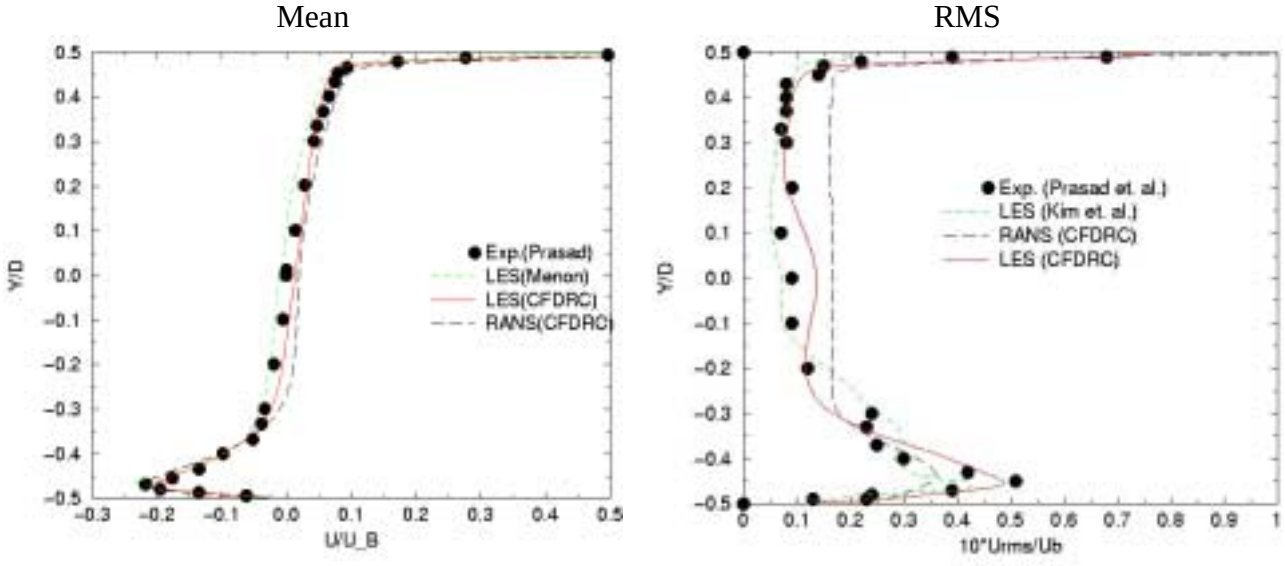


Figure 5. Normalized Mean and RMS U-Velocity

Linear Eddy Model (LEM) Implementation

Model Description: The Linear Eddy Model (LEM) for describing subgrid chemistry was implemented and tested in the unstructured CFD-ACE+ flow solver. The LEM describes the effects of turbulent stirring, molecular diffusion, and chemical reaction at scales down to the molecular level where reaction ultimately occurs. The LEM achieves this by subdividing each LES cell into a smaller one-dimensional domain. Along the one-dimensional domain, molecular diffusion and chemical reaction are treated explicitly. The influence of turbulent convection is modeled stochastically by random rearrangements of the scalar field along the domain. Each event involves spatial redistribution of the species field within a specified segment of the linear domain. For high Reynolds number turbulence described by a Kolmogorov cascade, these redistribution events can be obtained from appropriate scaling laws (McMurtry et al., 1992).

The LEM subgrid mixing and reaction processes are coupled to the large-scale transport in CFD-ACE+ through the LES resolved flux at each grid cell face through splicing events. Portions of the linear eddy domain are transferred to neighboring grid cells, as shown in Figure 6. These splicing events occur at a frequency determined by the large eddy time step and is much greater than the time step governing the convection-diffusion-reaction process in the subgrid.

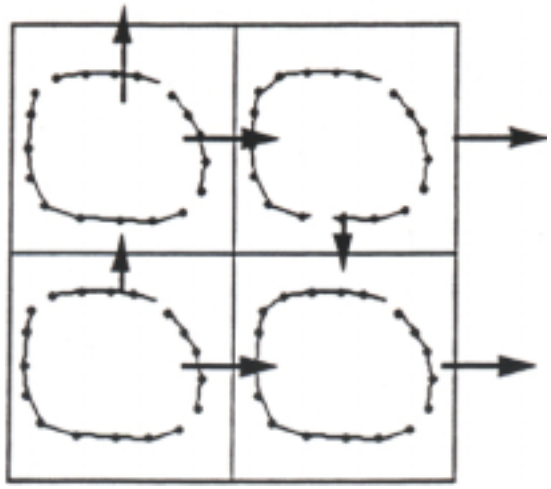
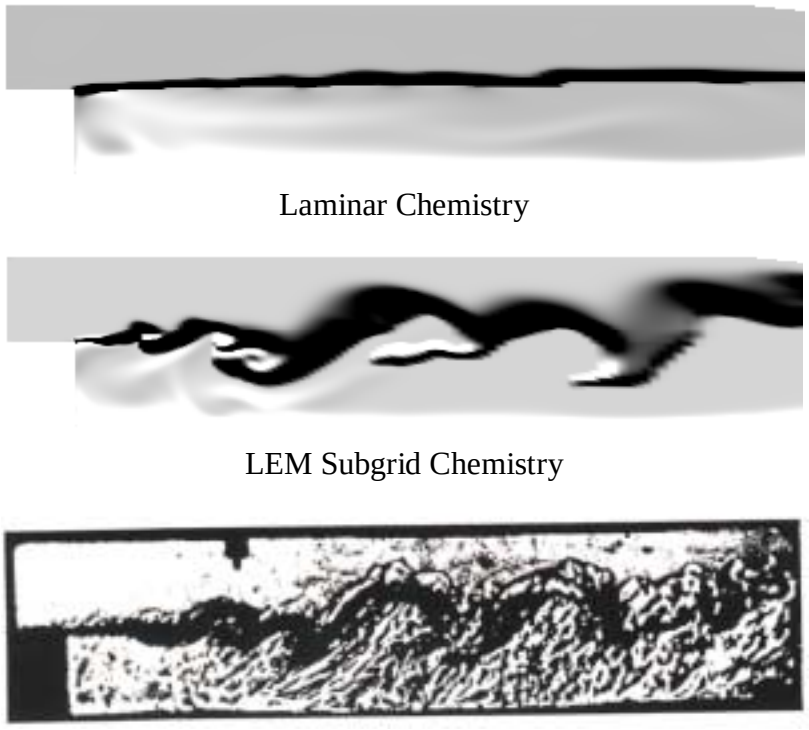


Figure 6. Schematic Diagram of the Linear Eddy Splicing Events

LEM Validation: The LEM was validated against experimental data from the reacting back-step case of Pitz and Daily (1983). The geometry, conditions, and results for the cold flow case were presented earlier. The reacting flow case utilized a premixed propane-air flame with an equivalence ratio of 0.57. Reacting flow simulations were carried out using a 1-step propane-air reaction with LEM. The LDKM subgrid turbulence model was used to close the momentum equations at the LES grid level and the subgrid tke provided necessary input for the LEM. For computational efficiency, these initial predictions utilized a 2D planar geometry. A total of 10,132 cells were used with clustering in the shear layer. Wall temperatures were specified according to the experimental data. A converged steady-state solution was utilized as the initial condition for the LES calculations.

The predicted instantaneous flame shape strongly depends on the subgrid chemistry model assumptions. Figure 7 shows instantaneous schlieren images for LES predictions using laminar chemistry and LEM and the measured Schlieren image. The laminar chemistry assumption did not account for subgrid stirring events and was not able to predict large-scale mixing. The LEM results showed significantly more large-scale mixing, in reasonable agreement with the experimental data. The very fine-scale structures do not show up in the predictions since their effects were described with the subgrid turbulence model.



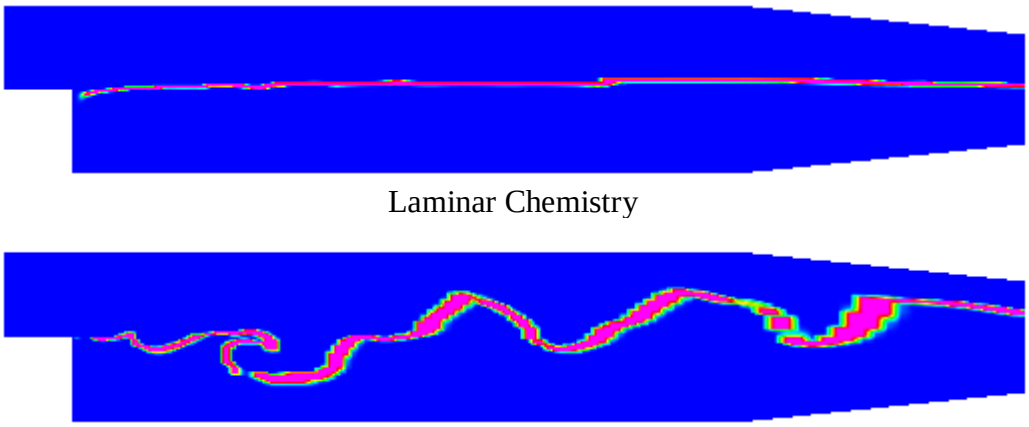
Laminar Chemistry

LEM Subgrid Chemistry

Measured Schlieren Image

Figure 7. Schlieren Images for LES Predictions and Measurements

In this reacting case, the incoming fluid contains cold premixed reactants which mix with hot combustion products in the initial shear layer behind the step prior to burning. The high turbulent strain rates (modeled in the subgrid) should delay the heat release, allowing the development of a Kelvin-Helmholtz instability. With laminar chemistry, the flame speed is independent of strain rate, and strong chemical reaction is allowed to take place immediately after the cold premixture contacts the hot products. The heat release in the shear layer inhibits the growth of the instability, resulting in a near smooth flame surface with very little wrinkling. The LEM includes subgrid turbulent stirring effects and allows the development of a Kelvin-Helmholtz instability. Figure 8 shows the instantaneous chemical reaction rates for the laminar chemistry and LEM predictions. Not only is the reaction zone delayed downstream of the dump plane for the LEM, but also the reaction flame zone is much wider at certain points and broken in certain points due to subgrid turbulent stirring.

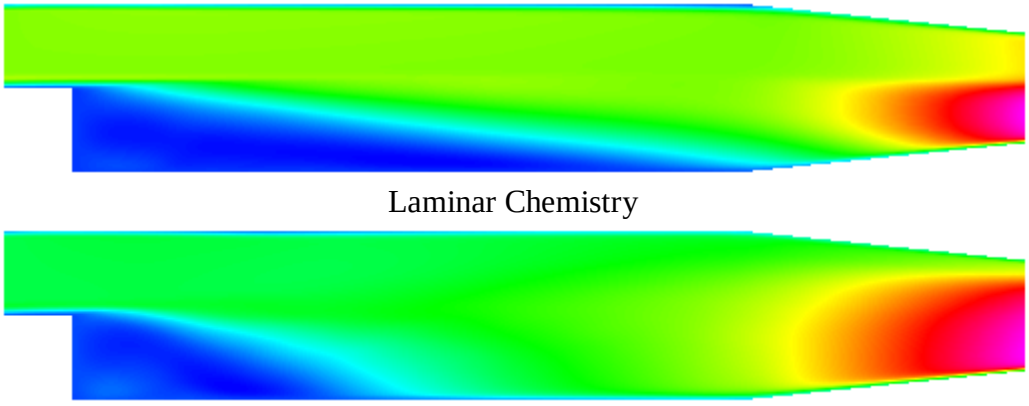


Laminar Chemistry

LEM Subgrid Chemistry

Figure 8. Predicted Chemical Reaction Rates

The reattachment length for the reacting flow is much less than the non-reacting case. Figure 9 shows the predicted reattachment length for the laminar chemistry and LEM predictions. The LEM case predicts a value of 3.6H, near the experimental value of 4.5H. The laminar chemistry prediction shows a reattachment length of almost 7.4H. The development of the shear layer vortices are required so the large-scale structures can close down the recirculation zone. These results show the need for accurate subgrid chemistry modeling, particularly in regions where strain rate extinction can occur. The LEM is now being tested in the full 3D geometry and with more detailed chemistry.



Laminar Chemistry

LEM Subgrid Chemistry

Figure 9. Predicted Time-Averaged Axial Velocity Contours Showing Reattachment Lengths using Laminar Chemistry and Linear Eddy Model

The computational time for the LEM subgrid and laminar chemistry model were similar. One reason for the relatively fast LEM is due to computing subgrid chemistry once per timestep, instead of at each iteration (7/timestep) for the laminar case. These calculations were performed with a fixed LEM cell number (32) in each LES cell. The effect of this LEM cell number needs to be

investigated. Overall these results are very promising, but further work with multi-step chemistry needs to be performed.

Linear Eddy Model (LEM) with Artificial Neural Nets (ANN)

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. Figures 10a and 10b shows the instantaneous and time-averaged 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.

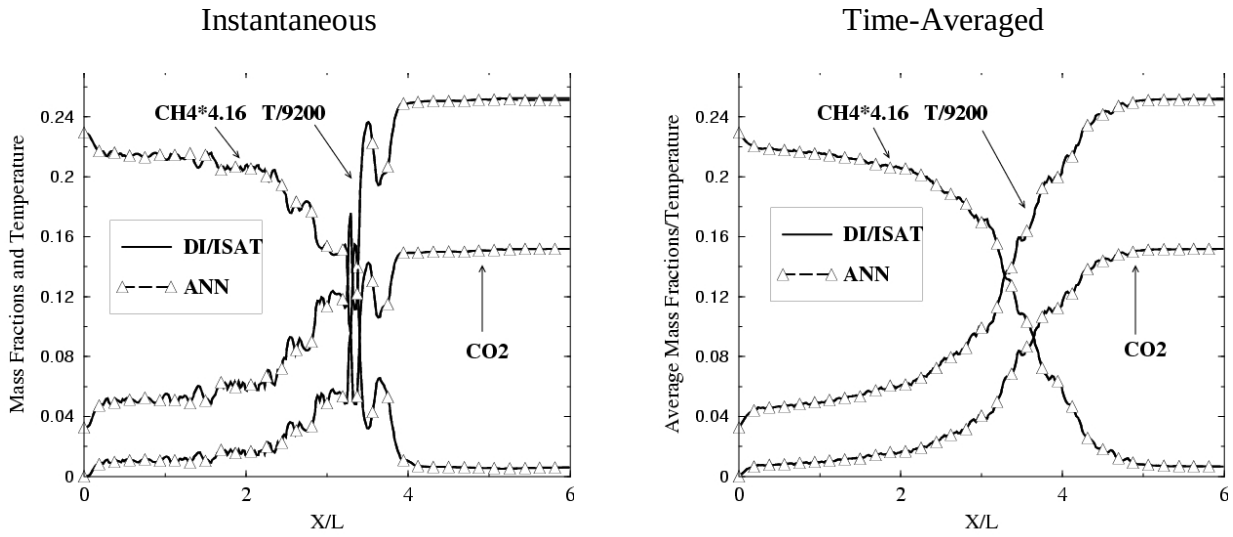


Figure 10. Instantaneous Flame F2 Profiles Predicted by Combining 2 ANNs (for F1 and F3). Results compared to direct integration by ISAT.

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.

Parallel improvements were applied to the transient lid driven cavity case. 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 11 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.

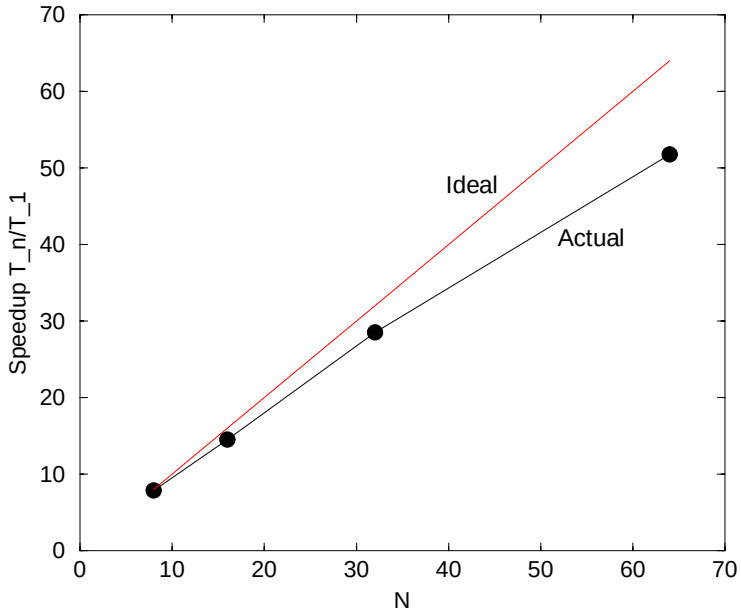


Figure 11. Speedup vs. Number of Processors

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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