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

**Quarterly Technical Progress Report for**

**January 2002 - March 2002**

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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 sixth quarterly report. CFD Research Corporation (CFDRC) is developing the LES module within the parallel, unstructured solver included in the commercial CFD-ACE+ software. In this quarter, in-situ adaptive tabulation (ISAT) for efficient chemical rate storage and retrieval was implemented and tested within the Linear Eddy Model (LEM). ISAT type 3 is being tested so that extrapolation can be performed and further improve the retrieval rate. Further testing of the LEM for subgrid chemistry was performed for parallel applications and for multi-step chemistry. Validation of the software on backstep and bluff-body reacting cases were performed. Initial calculations of the SimVal experiment at Georgia Tech using their LES code were performed. Georgia Tech continues the effort to parameterize the LEM over composition space so that a neural net can be used efficiently in the combustion LES code. A new and improved Artificial Neural Network (ANN), with log-transformed output, for the 1-step chemistry was implemented in CFDRC's LES code and gave reasonable results. This quarter, the 2nd consortium meeting was held at CFDRC.

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. Optimization of subgrid models will be pursued, particularly with the ISAT approach. Also next quarter, the demonstration of the neural net approach, for multi-step chemical kinetics speed-up in CFD-ACE+, will be accomplished.

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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 has 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. Now, in the second year, the combustion LES software will be evaluated and validated using experimental data from lab-scale and industrial test configurations, including important benchmark data from DOE-NETL. During the last year, seven 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 sixth quarter (January - March 2002) has included further testing of the Linear Eddy Model (LEM) in CFD-ACE+ for predicting subgrid multi-step chemistry. Also, In Situ Adaptive Tabulation (ISAT) for efficient multi-step chemistry has been further tested and refined. Georgia Tech continues efforts to train a neural net for accurate and efficient chemistry descriptions in the LES software. Initial calculations of the SimVal experiment were carried out to help guide the experiments that will be a database for validating the LES code.

Next quarter, completion of the following tasks are planned:

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

2. Carry out initial validation of LES code for predicting emissions and instability in cases selected by the industrial consortium.

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

## 3. EXPERIMENTAL

No experiments were performed this quarter.

# 4. RESULTS AND DISCUSSION

## 4.1 Selection of Validation Cases

Experimental data from four combustor cases were elected by validating the combustion LES software. The cases were partially selected by evaluating feedback from the industrial consortium. The four cases include:

- Taurus 60 fuel injector for industrial gas turbines (geometry and conditions provided by Solar Turbines, Inc.).
- Lean premixed methane-air bluff-body combustor (Vanderbilt and Sandia, Nandula et al., 1996).
- Lean premixed propane-air back-step combustor (Pitz and Daily, 1983).
- DOE-NETL SimVal combustor (Maloney, 2002).

The cases include transient pressure measurements for evaluation combustion instability predictions and detailed temperature and species measurements for validating emissions predictions. The cases include atmospheric conditions of interest to burner/boiler manufacturers and high pressure conditions of interest to gas turbine engine companies. Initial validation studies have been performed and are included in Sections 4.3, 4.5, and 4.6.

## 4.2 In Situ Adaptive Tabulation (ISAT)

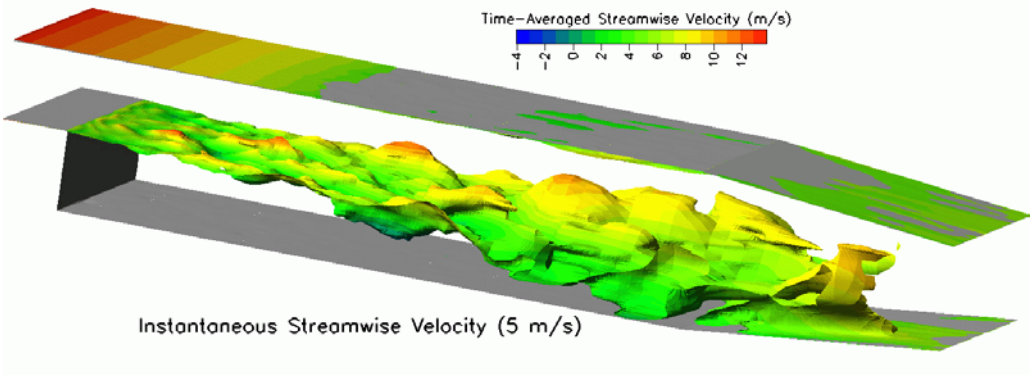
The In Situ Adaptive Tabulation (ISAT) algorithm for efficient treatment of multi-step chemistry has been implemented and tested in the LES code. Work shown in previous quarterly reports was limited to the laminar chemistry method. During this quarter, ISAT was implemented and tested with the LEM option for a more accurate description of turbulence-chemistry interactions at the subgrid level. Since, the diffusion-reaction time-step in LEM is computed locally on the fly, it was not possible to use the original fixed time-step ISAT. This required storage and retrieval of instantaneous reaction rates instead of integrated reaction increments. Also, the method for computing the sensitivity matrix needed to be modified since the DVODE solver was no longer utilized. As described in earlier reports, the sensitivity matrix is needed to provide $1^{st}$-order extrapolation within the ellipsoid of accuracy for a node in composition space. To date, ISAT type 1 and 2 have been implemented and tested with LEM. A 92% retrieval rate has been achieved for the 2D backstep test case using the 5-step methane-air mechanism and the 19-step propane-air mechanism. A bluff-body stabilized flame case has achieved only a 70-80% retrieval rate when using 5-step methane-air chemistry with LEM-ISAT. ISAT type 3 is now being tested so that extrapolation can be performed and potentially further improved the retrieval rate (i.e., reduce direct calculation).

## 4.3 On-Line Linear Eddy Model (LEM) Implementation and Testing

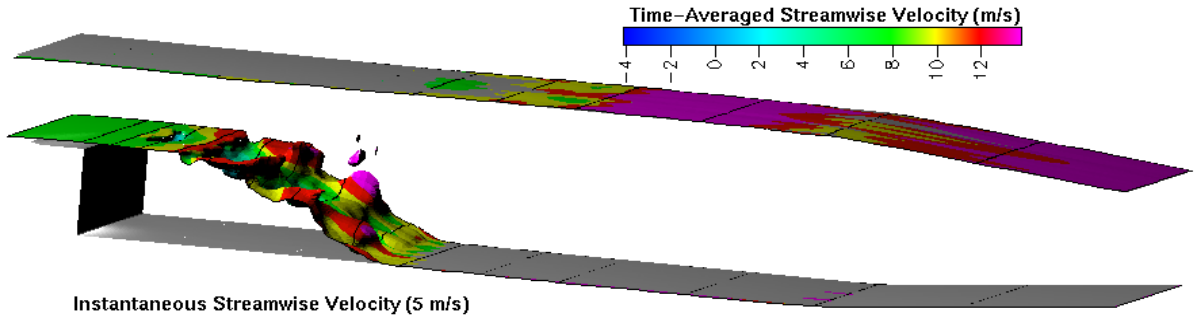
The Linear Eddy Model (LEM) for describing subgrid chemistry was implemented and tested in the unstructured CFD-ACE+ flow solver. The LEM describes the effects of turbulent stirring, molecular diffusion, and chemical reaction at scales down to the molecular level where reaction ultimately occurs. The LEM achieves this by subdividing each LES cell into a smaller one-

dimensional domain. The details of the LEM formulation were presented in the last quarterly report.

The LEM was validated against experimental data from the reacting back-step case of Pitz and Daily (1983). Figure 1 shows a calculated axial velocity isosurface for the (a) isothermal and (b) reacting flow cases. The recirculation zone has been properly predicted, with the length of the recirculation region X=7.2H for isothermal and X=3.8H for reacting flow. The LEM was needed to predict the shorter reattachment length for the reacting case. The laminar chemistry assumption did not allow a Kelvin Helmholtz instability to develop and thus large-scale vortex structures downstream of the backstep were not formed and a much longer reattachment length (7H) was predicted.



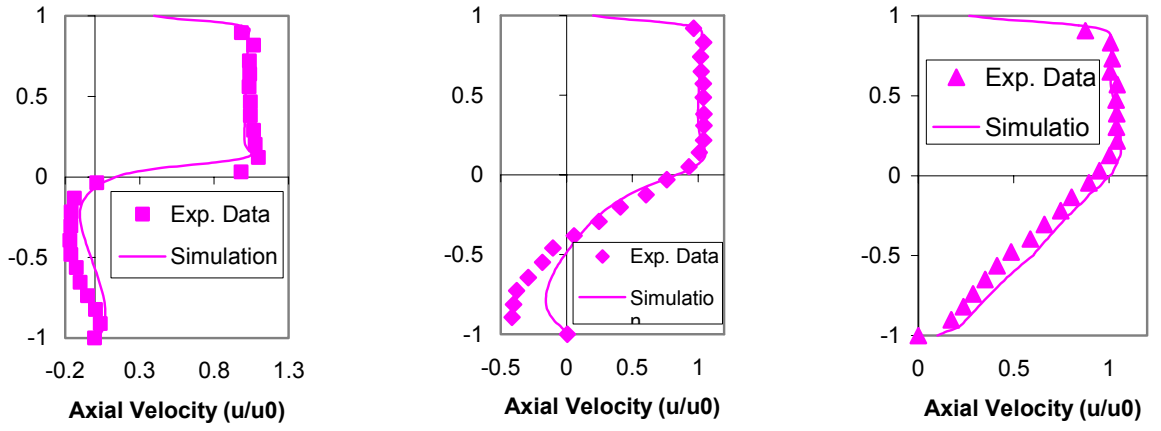

(a) Isothermal Flow




(b) Reacting Flow

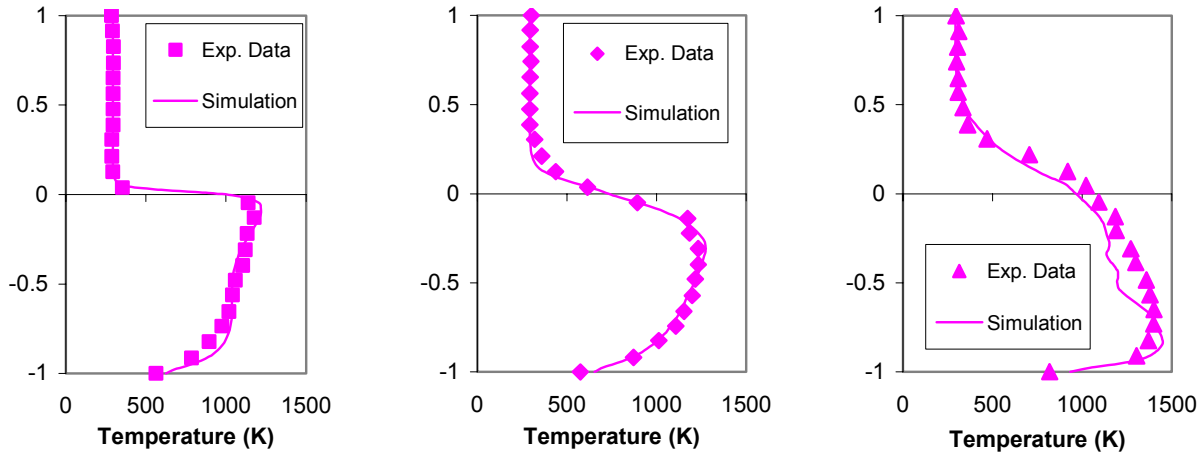
*Figure 1. Predicted Axial Velocity Iso-Surface for (a) Isothermal Flow and (b) Reacting Flow*

Detailed comparisons of experimental and predicted (using LEM) profiles of the mean axial velocity and temperature are shown in Figures 2 and 3. These results show good agreement between measurements and predictions. Radiative heat transfer was required in the model to obtain good agreement with measured peak temperatures downstream of the backstep. The most significant discrepancy was found for the velocity in the recirculation region at X=3H. At this location, the negative flow is underpredicted and was also observed in the non-reacting simulations. This effect could be due to the thick boundary layer at the side-walls which allows higher negative flow velocity on the centerline. This 3-dimensional effect was not modeled since the computational domain covered a Z distance of only 3H (with cyclic boundaries), rather than the full 6.5H with side-walls.




(a) (b) (c)

*Figure 2. Mean Profiles of Axial Velocity at (a) X=H, (b) X=3H, and (c) X=5H for the Reacting Backstep Case (simulations with LES+LEM)*




(a) (b) (c)

*Figure 3. Mean Profiles of Temperature at (a) X=0.4H, (b) X=1.2H, and (c) X=3.5H for the Reacting Backstep Case (simulations with LES+LEM)*

The LEM has been extended to work with In Situ Adaptive Tabulation (ISAT) for multi-step chemistry. This capability has been tested using both a 5-step methane-air mechanism and a 19-step propane-air mechanism developed by Prof. J.-Y. Chen. A 92% retrieval rate has been achieved for the propane-air 19-step mechanism. Unfortunately, the reacting flow for the backstep case blew out while using the LEM with 19-step propane chemistry. Details of the LEM algorithm are currently under investigation. Currently, at the end of the LEM algorithm for each LES time step, the 1D LEM cells are averaged together to form a mixture composition (temperature, density, and species mass fractions) that are passed to the LES cell centers. Then, also at the beginning of the next LEM computation, the averaged mixture for the LES cell center is divided evenly and assigned as the initial composition for each LEM cell. The molecular level resolution is lost and could be important for small concentrations of radical species that have a large influence on reaction. This potential problem is being corrected, as the individual identity

of each LEM cell is stored and not lost during the LES solution of velocity, pressure, and enthalpy.

In addition to multi-step chemistry, efficiency improvements have been implemented into the LEM algorithm. The LEM cell number is now computed locally at each global LES timestep as a function of the local, instantaneous dissipation scale. Also, in regions with minimal reaction, the LEM cell number is kept low. Improvements to the LEM algorithm have also included the ability to handle 2d axisymmetric grids.

### 4.4 Off-Line Linear Eddy Model Using Neural Nets

Laminar Artificial Neural Networks (ANN) have been successfully developed at Georgia Tech for the single step Westbrook-Dryer mechanism for methane-air combustion. The present laminar ANN development uses a completely different approach using a training set that involves point-evolution of the chemistry for a given input set of conditions ($\Phi$=1.0; T=300K, P=1atm). This laminar ANN is then tested on a 2D DNS code, and the results are compared with direct integration (DI). This is done for both a laminar flame problem and for a turbulent flame problem (with specified inflow turbulence conditions). The progress in the development of the ANN for the 15-step, 19species $CH_4$ mechanism is also discussed.

The evolution of a laminar flame is simulated and evolved in time. The training set for the ANN is chosen from this setup. 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 in a much more efficient manner since it eliminates any biasing of the sample points in any temperature range. Figure 4 shows a typical profile of one of the outputs of training. As seen from the figure, an ANN trained for the entire temperature range will be highly error prone due to the non-linearity depicted by the output. Thus, some kind of conditioning is should make the training easier and more accurate. A logarithmic transformation is performed for the output variables and shown in Figure 5. As can be seen, the output set that is to be used for training has become more uniform over the temperature range of operation.

Laminar ANN for the single step 5 species methane-air mechanism is developed using this concept. Figure 6 show the typical profiles as obtained using the laminar ANN versus a direct integration simulation (in a 1D standalone simulation). Clearly, excellent agreement between the two methods is achieved in the training exercise.

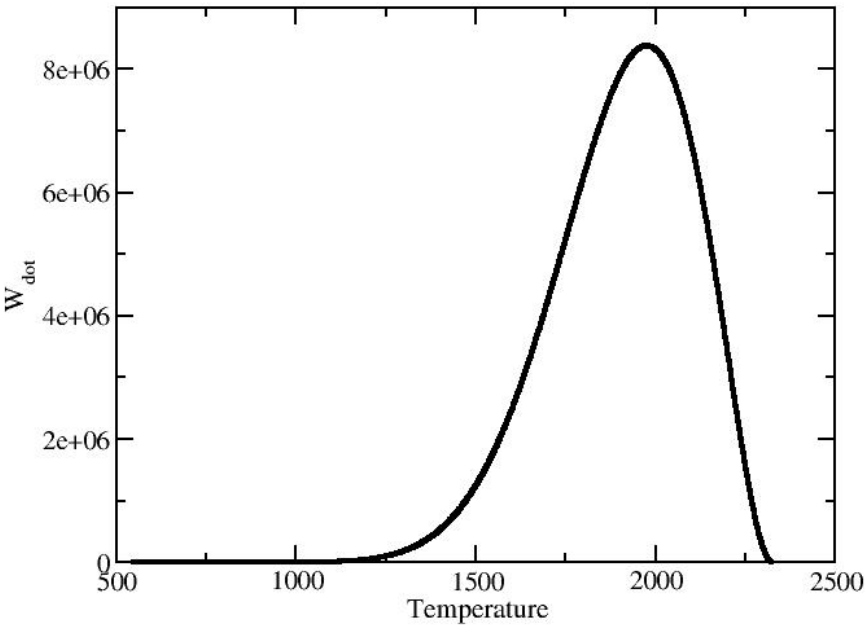



*Figure 4. $(Y_2-Y_1)/dt$ vs. Temperature*

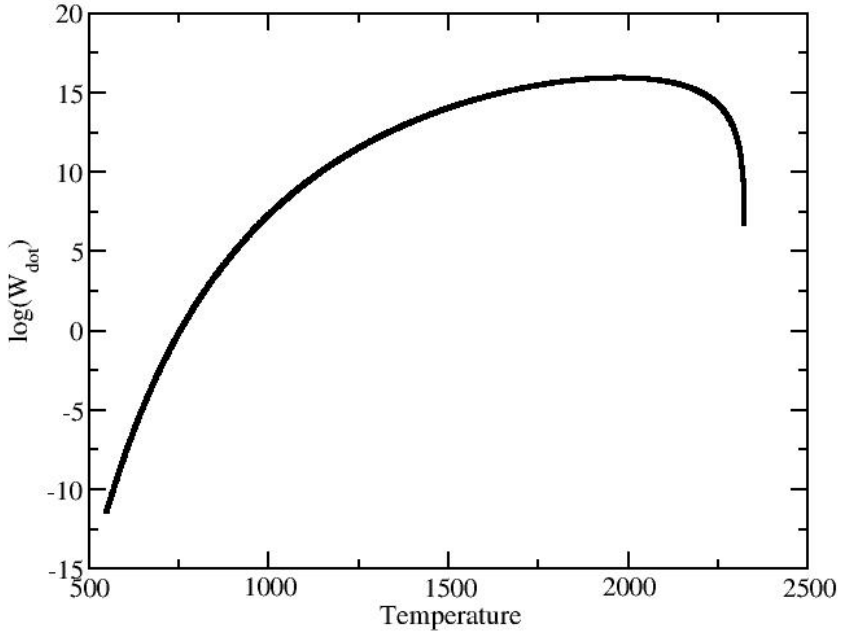



*Figure 5. Log $[(Y_2-Y_1)/dt]$ vs. Temperature*

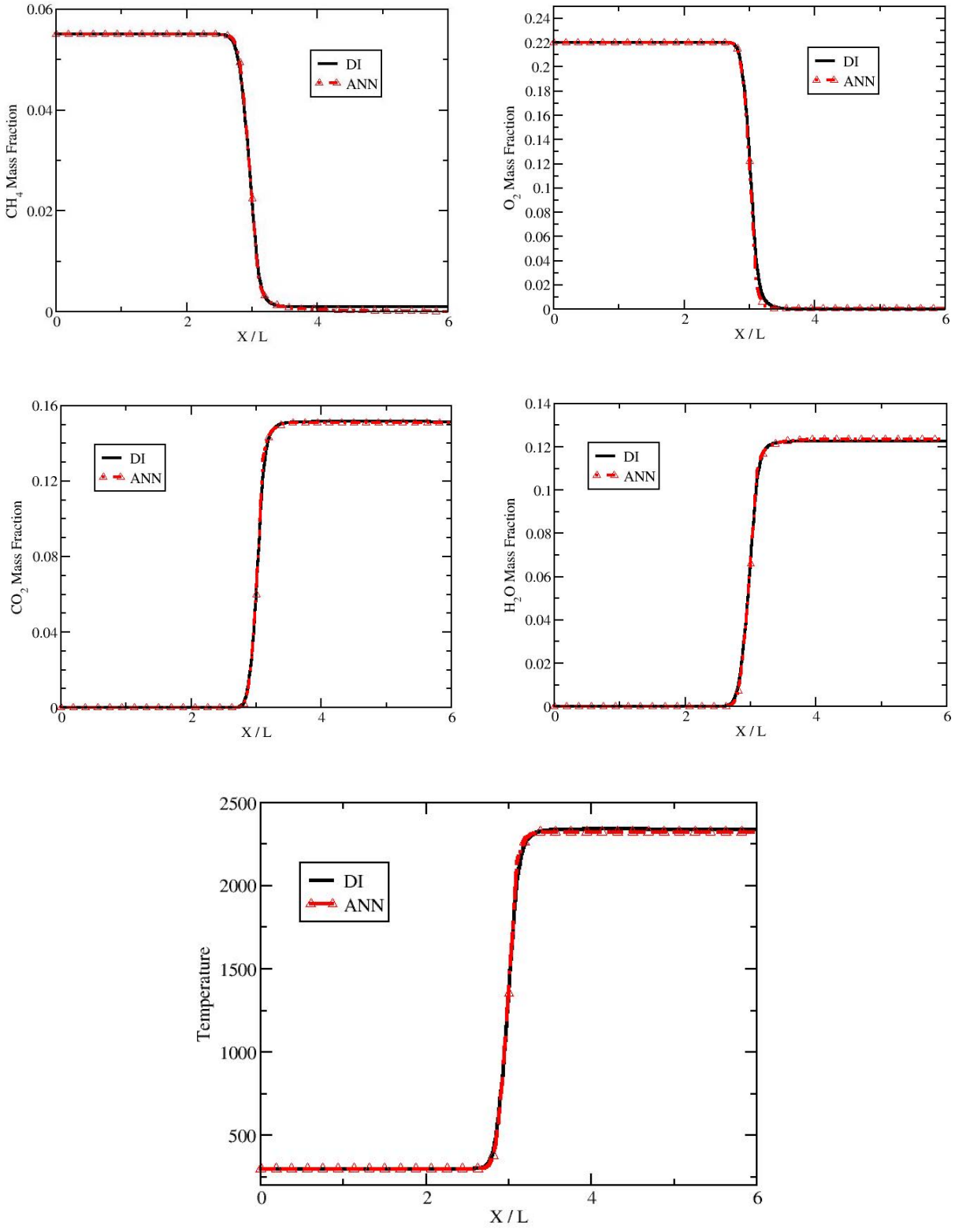



*Figure 6. Scalar Profiles for Species/Temperature (ANN vs. DI)*

## 2D DNS of Laminar Propagating Flame

The developed laminar ANN is implemented in a 2D DNS code and the results compared against the results from direct integration. A very high grid resolution of 400x400 is used to resolve a computational domain of (0.025m x 0.025m). The simulation is conducted with a laminar flame profile initialized in the middle of the domain. Inflow and outflow boundary conditions are prescribed using characteristic wave directions. At the inflow, a velocity for the premixed mixture is prescribed with a reference velocity of 0.4m/s (≈ laminar flame speed for stoichiometric methane mixture). With this initialization, the laminar flame should remain at approximately at its initial location for the entire simulation.

Figure 7 show the typical results obtained for the same using laminar ANN. Figure 8 shows the comparisons for the same against a similar DI option. As can be seen, the profiles for the two approaches match in excellent agreement with each other. Furthermore, the flame remains flat and stationary, indicating that the laminar flame has been properly resolved and captured using both the DI and ANN approaches.

Subsequently, DNS of the same case is carried out using an isotropic turbulent field prescribed in the domain and now, the flame is allowed to interact with the turbulent flow field. The inflow is also modified to bring in an isotropic turbulent field at every time-step. The grid resolution and domain is used here (as in the laminar case) with a mean inflow velocity of 0.4m/s and a fluctuating velocity $u_{rms}$ = 1.77m/s. Figures 9 and 10 show some typical results from the simulation with the ANN. Both DI and ANN calculations show nearly identical wrinkled flame structure. The effect of heat release on the flow structures behind the flame is to diffuse the structures and this effect is also resolved in the simulations.

Analysis of the results shows that ANN has been successfully implemented in the DNS code and has been used to resolve the flame. Application in both laminar and turbulent cases show that this approach is stable and accurate. Furthermore, ANN proved to provide a speed-up of the order of 5 over the conventional DI case (e.g. time/step: DI ≈ 0.3685sec; time/step ANN ≈ 0.0746sec). This speedup is expected to be even higher (by orders of magnitude) when a more detailed chemistry (e.g., 19 species) is employed due to the increased stiffness of the DI (or ISAT) approach. The memory requirement for ANN is also expected to be orders of magnitude less than for a similar ISAT run. At present, the ANN memory requirement is about 1.2 MB, which is only marginal compared to ISAT storage requirements (which can be up to 100 MB or more depending on the required ISAT accuracy).

## Work Under Progress

The above methodology is being extended and used to develop the 19-species ANN. Once developed, we plan to redo the DNS studies using the 19-species ANN to compare it with DNS using ISAT. These results will be reported next quarter.

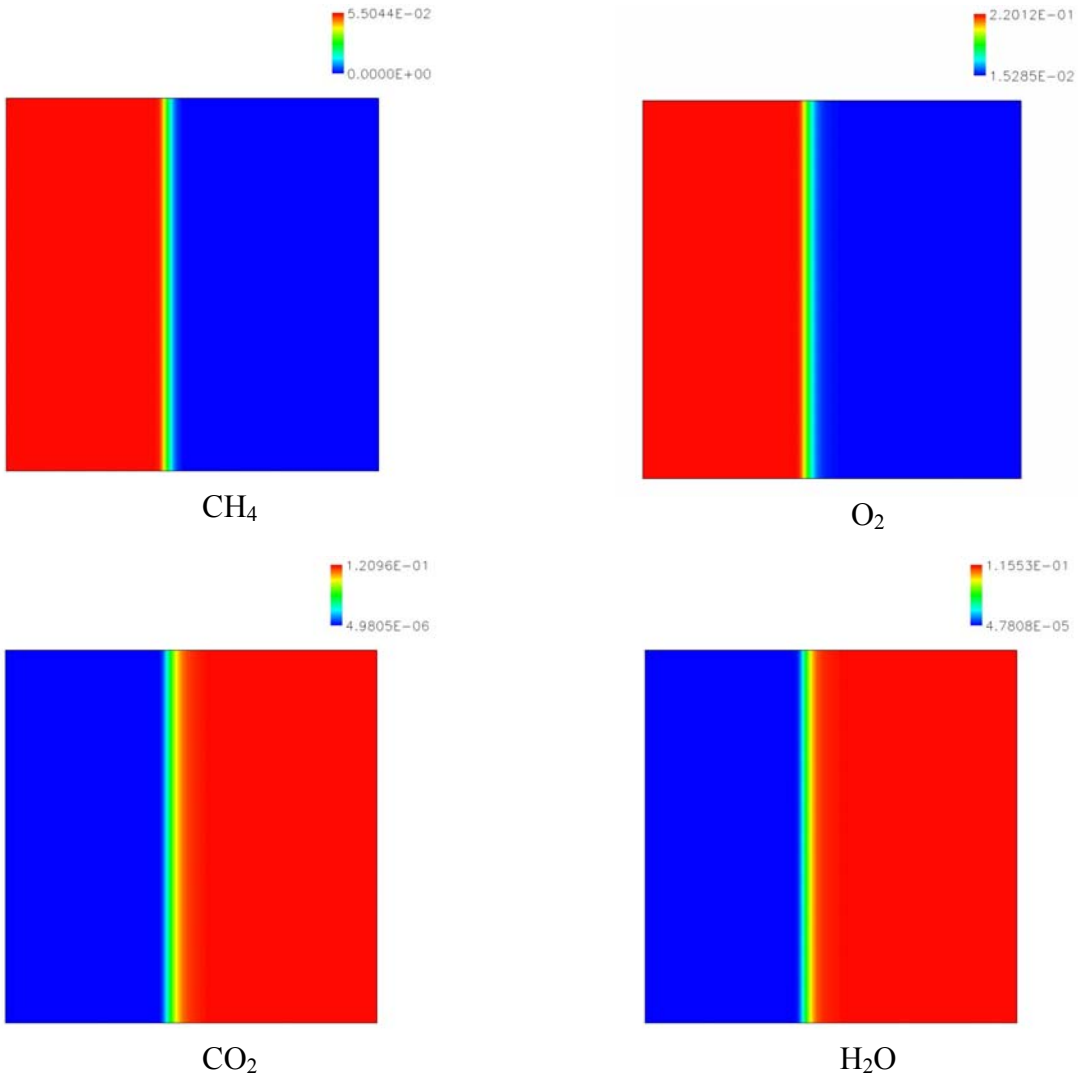



*Figure 7. 2D DNS Simulation with 5-species Laminar ANN*