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Large-eddy simulations (LES) of turbulent flames with detailed finite-rate kinetics is currently computationally infeasible due to the enormous cost associated with computation of reaction kinetics. Recently, an In-Situ Adaptive Tabulation (ISAT) methodology was shown to reduce the cost of direct integration considerably. However, ISAT tables require significant on-line storage in memory and may result in restriction on massivelly parallel systems. Furthermore, application of ISAT in LES requires re-evaluation of the tree structure and the access/retrieval process. Here, issues regarding the use of ISAT in a LES are discussed. Then, a storage-efficient Artificial Neural Network (ANN) is trained using ISAT data and used to simulate turbulent premixed flames in both the thin-reaction-zone and flamelet regimes. Finally, the issues to be addressed in order to apply this combined ISAT/ANN methodology for full-scale LES of reacting flows are discussed.

1 Introduction

Recent more stringent emission regulations have pushed for the development of more efficient and low-NO_x gas turbine systems. Accurate prediction of mixing and combustion processes, including pollutant emission in such systems requires a comprehensive numerical model that can predict flame structure and propagation characteristics, formation of both major and minor chemical species, and ignition/extinction phenomena over a wide range of flow conditions in high Reynolds numbers. Direct numerical simulations are not practical, since the resolution and computational resource requirement far exceed the present and near future computational capabilities. On the other hand, steady state methods are not acceptable, since they only predict mean motion and properties of the flow using a global averaging approach, and therefore, are unable to capture the unsteady dynamics.

An approach that can address both the unsteady dynamics of the flow and the turbulence-chemistry interactions accurately is the method developed recently

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that combines conventional LES for the momentum transport with a subgrid simulation model to capture the local reaction-diffusion processes.[1-7] In particular, the key features of this subgrid model is that both reaction kinetics and molecular diffusion processes are implemented exactly as in a local direct simulation. In addition, since the advection of the subgrid fields is carried out using a Lagrangian transport model, the transport of the subgrid scalar fields across LES cells is accomplished without requiring conventional differencing, and as a result, both co- and counter-gradient diffusion process at the resolved scales are captured without requiring ad hoc models. Further details of this subgrid combustion modeling approach is given elsewhere in the above cited papers.

In order to predict flame extinction/reignition and pollutant formation, detailed reactions kinetics have to be simulated within the LES model. This can be computationally prohibitive due to the cost of direct integration of the chemical kinetics. Methods developed in the past using the mixture fraction and the G-equation model are limited by the inherent assumptions in these types of formulations (e.g., equal diffusivity, two-feed systems, etc). Furthermore, for practical gas turbine engines where both pilot and secondary flame zones are employed (for both stability and efficiency), the mixture fraction approach is inapplicable due to the formation of multiple premixed, partially-premixed and non-premixed zones. Thus, LES of chemical kinetics in realistic combustors will require a new approach that is not only computationally efficient but also accurate.

Earlier simulations using the subgrid model have already shown good results in the flamelet regime when coupled to a G-equation model[1,2,8] or on a single step mechanism.[4,9] LEM calculations with finite-rate chemistry implemented with ISAT have proven to capture reasonably well the physics for different regimes of premixed combustion.[10] However, ISAT requires significant storage (in memory) that increases with the number of species and the chemical composition space. Since all LES have to be carried out on massivelly parallel systems (including PC clusters), the local memory overhead of ISAT can become a bottleneck when used for large-scale simulations. Therefore, an
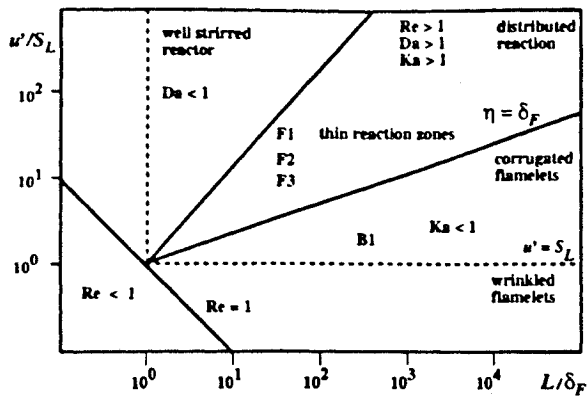
Fig. 1 Diagram of turbulent premixed combustion regimes.

alternate method based on artificial neural networks (ANN) for the prediction of the evolution of the scalars in the fluid flow is investigated and demonstrated in the present effort. Earlier, Haykin[11] noted that ANN is a massively parallel distributed processor made up of simple processing units, which has a natural propensity for storing "experience" knowledge and making it available for use. The present study exploits this ability to study reacting flows with finite-rate kinetics.

The use of ANN is widespread in the engineering community, but is relatively novel in combustion related CFD applications. Some of the past work worth mentioning[12-14] and more recently[15] all addressed the ability of ANN to accurately map the composition space. In the present work, the ANN approach is used to simulate a turbulent premixed flame with a 19-species, 15-steps methane-air mechanism.[16] The temporal evolution of any reactive scalar is given in the form

$$\frac{dy_i}{dt} = \dot{\omega}_i(y, T, P) \tag{1}$$

The energy equation can also be written in a similar fashion for the temporal variation of temperature in the system. A stand-alone Linear Eddy model (LEM) developed earlier[10] is used for ANN training and simulations. The current effort focusses on the ability of "off-line trained" ANN (as opposed to an "on-line" ISAT or DI) to capture the details of the chemical composition in a high-Re turbulent flame. In particular, the ability to build ANNs that cover a wide range of premixed flame characteristics as in the thin-reaction-zone and corrugated flamelet regime (Fig. 1) is investigated here. Future extensions to deal with parametrization of the thermo-chemical and turbulent parameters within the ANN approach are also discussed.

2 *In Situ* Adaptive Tabulation for LES

The chemical reaction terms appear in closed form in the LEM equations. Employing operator splitting for diffusion and reaction terms, the latter are simulated by solving a stiff system of ODE's (Equation 1). Direct integration of such equations is prohibitively expensive, and would make LES-LEM simulations with finite rate chemistry unfeasible. Some approaches[17] resort to pre-calculation and tabulation of the thermochemistry. These tables store information about the thermochemical variables as a mapping from initial to final conditions in the integration of the stiff ODE's. However, there are some problems with the complexity of the interpolation, and most of all, storage requirements increase as the dimension of the problem grows. A relatively new tecnique called *In Situ* Adaptive Tabulation (ISAT)[18] has proven more efficient.

In ISAT, only the accessed region of the composition space is tabulated instead of the whole realizable region, i.e., only where the reactive flow computations occur. As ISAT builds its table only for the accessed region, the overall time required to build, retrieve and store information reduces significantly. Also, this tabulation can be done as the flow simulation proceeds, instead of earlier.

The new ISAT algorithm follows for most part the original algorithm by Pope.[18] Reactive flow calculations provide the ISAT code with the time step δt, a set of initial thermochemical parameters and variables to be updated. This initial chemical state is called "query composition". A closest neighbor search is performed in the table to determine which of its points best matches such initial chemical state. The data structure employed for the table is of paramount importance for the success of such search, especially for LES.

The data structure used in the original ISAT code is a multidimensional binary tree that divides the composition space with hyperplanes. A query performs a search from top to bottom of the tree moving down its branches to the left or right of its nodes according to which side of the hyperplane it is located. At the bottom it reaches a record called "leaf", that is used for the retrieval operation, where the integrated solution is approximated and its accuracy assessed. This coupled data structure and search algorithm have shown some limitations, as only a single branch of the tree is searched and at times the closest neighbor search fails. This often leads to unnecessary extra direct integrations, as a new leaf is created each time the approximated solution is not found accurate enough, and also to some problems with memory requirements, as the size of the table increases.

In the new algorithm a more traditional k-d tree data structure[19] is employed where the hyperplanes that divide the region are held perpendicular to the

composition space. Nodes (and corresponding hyper-planes) in the tree are found by determining which of the coordinates among the records produces the largest (scaled) variance, allowing also the possibility of tree balancing and logarithmic search time. The search for the closest neighbor is also improved allowing the ISAT code to estimate all the branches that need to be viewed. This allows 100% rate of success in the search, and has shown to produce smaller tables. In simulations of F1 flame with a stand alone LEM code, it has produced tables as small as 25% of the size of tables from the original ISAT, given the same accuracy.

Also, a new feature has been added to allow the mapping from the initial state to average reaction rates, rather than the final state. This is especially important when very small time steps are taken, as changes in the chemical compositions can be smaller than the imposed accuracy. For incompressible time-accurate simulations, this is generally not an issue, with time steps hardly smaller than 10^{-5} sec. Also, for RANS applications, the time step is usually chosen for stability and not for time-accuracy and therefore, this is not an issue. However, for compressible LES studies (which are needed for real gas turbine flows where acoustic-vortex-flame interactions are critical, and have to be resolved), the time step is typically of the order of 10^{-7}-10^{-8} sec.

The use of ISAT in compressible flows produces another unwanted problem, which is the creation of very large tables, as compared to incompressible flow calculations. This is inevitable, as transients are more finely reproduced, increasing the size of the accessed region of the composition space, especially when differential diffusion is accounted for. The speed-up from ISAT is also decreased, since for smaller time steps, the computational time for the integration of the ODE's decreases, while the table size and therefore, the searching time increases. F1 flame simulations with a stand alone LEM code showed speed-up up to no more than 60, with a time step of 6×10^{-8} sec, based on diffusion. Pope reported speed-up up to 1000 for well stirred reactor simulations with time steps of the order of 10^{-4}.[18] However the new ISAT mitigates such problem by keeping the table from overgrowing.

3 Artificial Neural Network for LES

An ANN structure consists of large interconnected non-linear processing elements, which by definition, mimics the functioning of biological neurons possessed with the ability to learn from the set of input-output parameter space it is subjected to, and then, predict the outcome for any new input set with a sufficient level of accuracy. The information for the network is stored in the form of weights and biases, which are computed iteratively in the learning phase of the network training.

Figure 2 shows the structure of a basic three layer neural network that has been used for most of the current work. The basic steps for obtaining an ANN structure are (i) the generation of an initial dataset for training the network, (ii) the training of the network using a suitable neural net algorithm, (iii) the generation of a validation data set to check the accuracy of the final ANN for sample points not used in the training, and (iv) the incorporation of the ANN in a real turbulent flame simulation.

ANNs are constructed to predict the temporal evolution of the reactive scalars and temperature in the 1D LEM domain. The aim is to predict the species mass fractions and the temperature after a given time step, and for a given input species composition and temperature. The time step for the calculation of the chemical evolution is kept constant in the current simulations and varies in the range $\sim10^{-7}$ - 10^{-8} sec for the B1 and F1 flame, respectively (see Fig. 1).

Individual ANNs, as shown in Fig. 2, are constructed for each of the target 19 species mass fractions and temperature. Each of the ANN, however, takes all the 20 scalars as an input. This allows for a higher accommodation of the intrinsic non-linearities of the problem. Each ANN is a three-layer scaled conjugate gradient (SCG) back-propagation network,[20] with 20 neurons in each of the hidden layers. The choice of the number of layers and number of neurons in each layer is an open question, and has been optimized iteratively. The SCG algorithm used has proven to be quite robust and faster than the conventional ANN algorithms used elsewhere.[14] Tan-sigmoid activation functions are used for the hidden layers, and a purely linear activation function for the output layer is employed. The most challenging task in the creation of a neural network for a chemical system is the generation of the training set, which should represent the accessed composition domain faithfully. The present study, uses the aforementioned ISAT table as a training data-set. However, it is still not clear if this is the optimal solution. On the other hand, use of the ISAT data reduce the cost of on-line evaluation of the chemical composition.

Two successive linear transformations are performed on the input-output data-set, namely (i) standardizing the variable values to achieve zero mean and unity variance,

$$x_i' = \frac{x_i - \tilde{x}_i}{\sigma_{x_i}} \quad (2)$$

where x_i is the value of the input/output variable i (species mass fraction or Temperature) and $\tilde{x}_i$ and σ_{x_i} are the mean and variance of the same, respectively. x_i' is the standardized value of the variable x_i, and (ii) rearranging the input/output sets to fall in the [-1,1] interval. The normalized [-1,1] range has been proven to be an optimized range for the ANN training. Thus, a linear transformation has been applied to the initial
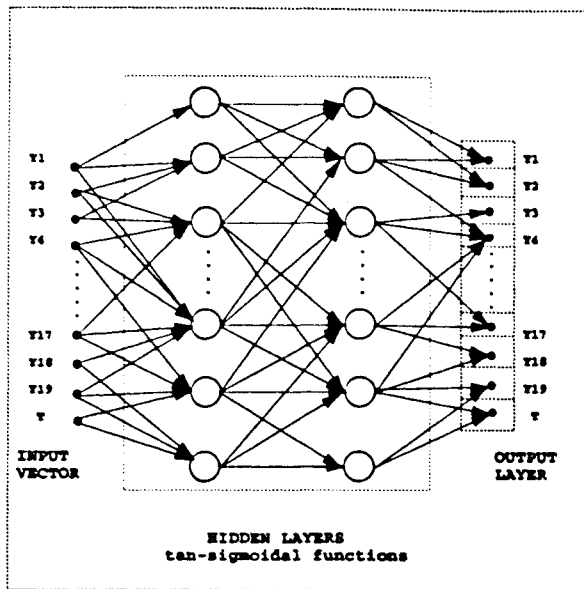
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Fig. 2 A three layer neural network structure.

data-set so as to allow it to fall in the above mentioned range.

4 Results and Discussion

The simulation model used to study premixed flames in the thin-reaction-zone and flamelet regimes[10] is used here to evaluate the performance of the new ISAT model and the ANN approach. The ANN structure is obtained after training is substituted for the calculation of the chemistry part, to predict the scalar evolution. Figure 3 shows some of the ANN predictions for the normalized scalars. As mentioned before, the SCG training algorithm provides excellent agreement for the predictions and these results confirm the accuracy of the training model.

However, the key issue for LES is the incorporation of these off-line trained ANN into the real flame simulation where other un-specified parameters/effects (e.g., flow, turbulent stirring,etc.) are also prevalent. As a result, the ANN training on a pure thermo-chemical composition space may not be sufficient to capture the overall dynamics of a turbulent flame. This issue is further complicated by the fact that the chemical mechanism consists of 19 species and the associated scalar evolution (Equation 1) is a highly non-linear problem. The overall data set used in the present work is highly skewed with a high probability of a particular target value for the scalars. This can viewed in the probability distribution function (Fig. 4) for one of the output scalars in the accessed domain of the flame region considered. In this figure, the x-axis denotes the instantaneous reaction rate for the scalar. Of course, the nature of the curve depends on other parameters, including the simulation time and the size of the intervals for constructing the PDF. However, a general trend can be inferred from the figure, which

is representative of the behavior of most of the output scalars in the problem. Such a data set is said to be ill-conditioned for ANN training process, and demonstrates the complexity involved in simulating finite-rate chemistry effects using ANN.

After the ANN is incorporated into a real flame chemistry problem, the predictions for the turbulent premixed flame considered are compared with those obtained by the direct integration (DI) approach for the chemical evolution of the species. Figures 5(a-d) show the instantaneous comparisons for some of the major and minor species (CH_4, CO, NO) and temperature, respectively, in the flame normal direction for the F1 flame. As observed earlier, the flame structure in the thin-reaction zone is broadened due to the interaction of eddies smaller than the flame thickness with the flame. This feature is captures quite accurately using both ISAT and ANN. As can be seen from the figures, the ANN is able to sufficiently represent the scalar evolution in the reacting system. The inability of the ANN to accurately capture some of the fine scale phenomena can be attributed to the inadequate representation of the composition space by the initial training set and the highly skewed nature of the output sample points. Work is currently underway to optimize the results in this aspect.

Figures 6(a)-(d) show the average scalar profiles for CH_4, CO_2,CO and NO for the same flame. Figure 7 shows the average profiles for some of the radicals, temperature and the reaction rate for CH_4. Clearly, although the ANN prediction follows the the variation of all species quite closely, there are still some errors in the overall "time-averaged" predictions. Analysis of the ANN behavior suggests that this might be due to the rather rapid variation in a small range of some of the key radicals in the flame zone. A new approach which further fine-tunes the ANNs in these regime is being developed to further optimize the prediction.

Prediction of the average species profiles using the ANN approach for the B1 flame are shown (figure 8 and figure 9). Due to the flamelet shape of the B1 flame, the training of ANN on this flame was found to be more difficult and small errors in the prediction of key radicals resulted in significant errors in the overall structure. Again, this suggests a fine-tuning of the ANN within a subset of the composition where rapid variations are occurring. A new approach which subdivides ANNs within a local composition space in now being tested to address this concern.

An extension of this approach is to include an additional ANN that contains turbulence parameters such as the subgrid intensity and range of turbulent eddies in the flame zone ($f(l)$). For example, the F1 and B1 flames have different u' and $f(l)$ and by combining ANNs for these flames with ANN for u' and $f(l)$, it will be possible to directly obtain the filtered reaction rates without resorting to direct integration. This would
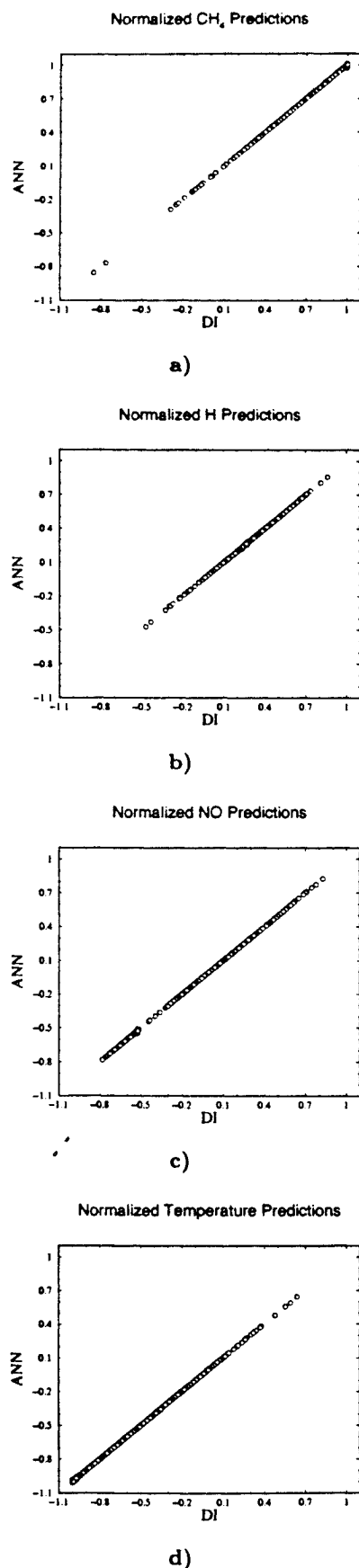
Normalized CH₄ Predictions

a)

Normalized H Predictions

b)

Normalized NO Predictions

c)

Normalized Temperature Predictions

d)

Fig. 3   Normalized off-line predictions of some of the scalars for the F1 flame ANN training.
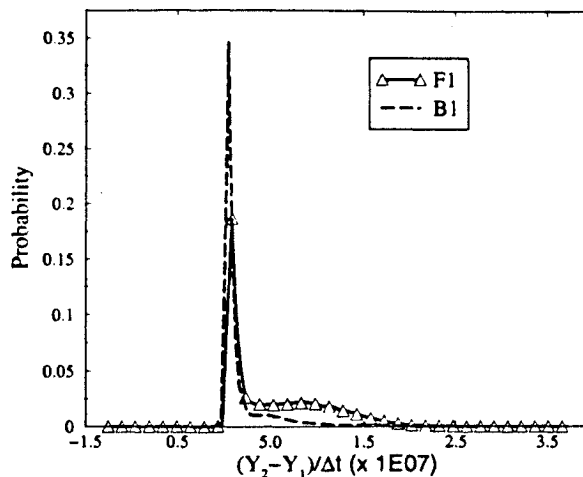

Fig. 4   PDF for one of the output scalars for the F1 and B1 flame considered.

allow inclusion of detailed kinetics into LES solvers without the associated (enormous) increase in computational effort. Such a study is currently underway and will be reported soon.

5   Error estimates and computational issues for ANN

The neural network algorithm is allowed to converge to a sufficient level of tolerance error. Mean square errors are used to define the overall network errors between the desired target value and the ANN predicted values. It is seen that convergence is more difficult to achieve for some of the radicals than the major species/temperature. Figure 10 shows the scatter plot for the network error that is obtained for one of the outputs in the F1 flame. As can be seen from the figure, most of the error in the predictions is close to the value of 0.0, which also happens to be the most probable value in this case. This may be argued to be one of the reasons for the slight offsets in the ANN predictions. With this deviation in context, overall the ANN proves to be an excellent competitor to represent finite-rate chemistry in a turbulent flame simulation. The major advantage it has to offer are in terms of the reductions in the computational costs and memory usage. Direct integration approaches are not always feasible, due to the enormous computational costs involved. For example, ISAT for the same chemical mechanism requires around 100-200 MB which has to be stored in memory to speed up access. On the other hand, the present ANN model (using 20 ANNs, one for each species and temperature) requires less than 1 MB of memory. This is significant implication for use within massivelly parallel systems (especially PC clusters) where the memory needs to be allocated to resolve for the flow field rather than for the chemical state.
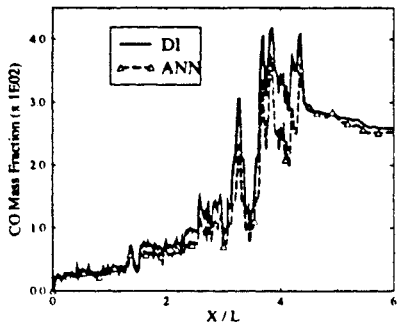
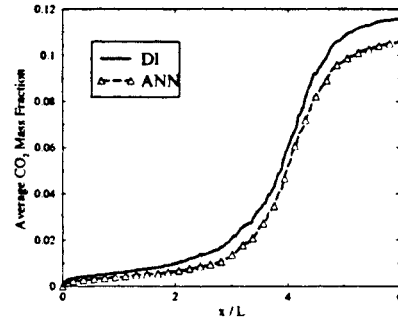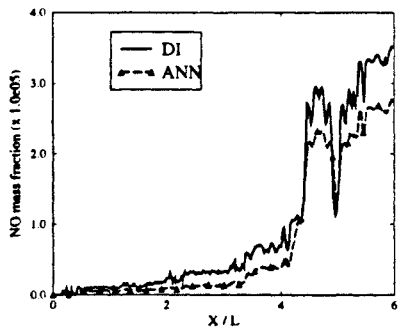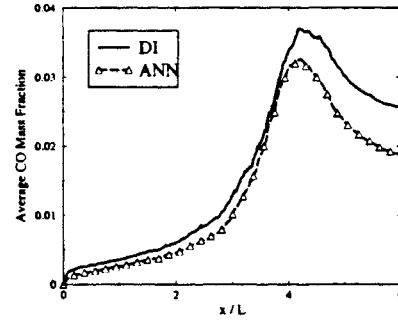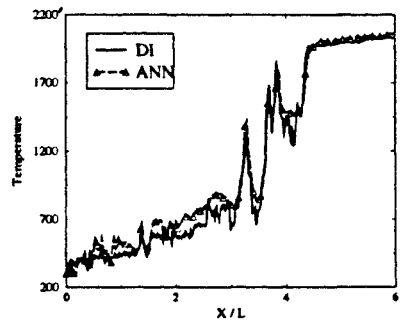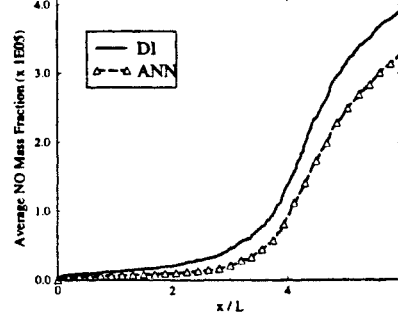Another issue is that ANN implementation is sim-
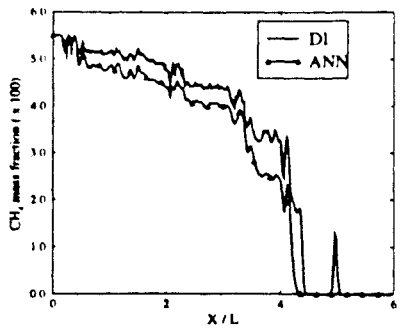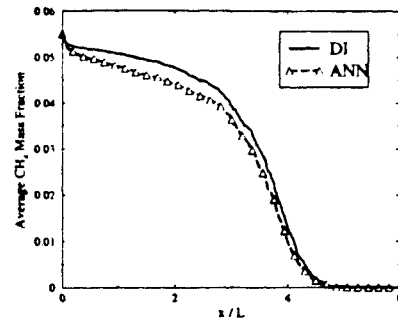
Fig. 5 Instantaneous scalar profiles for the F1 flame.

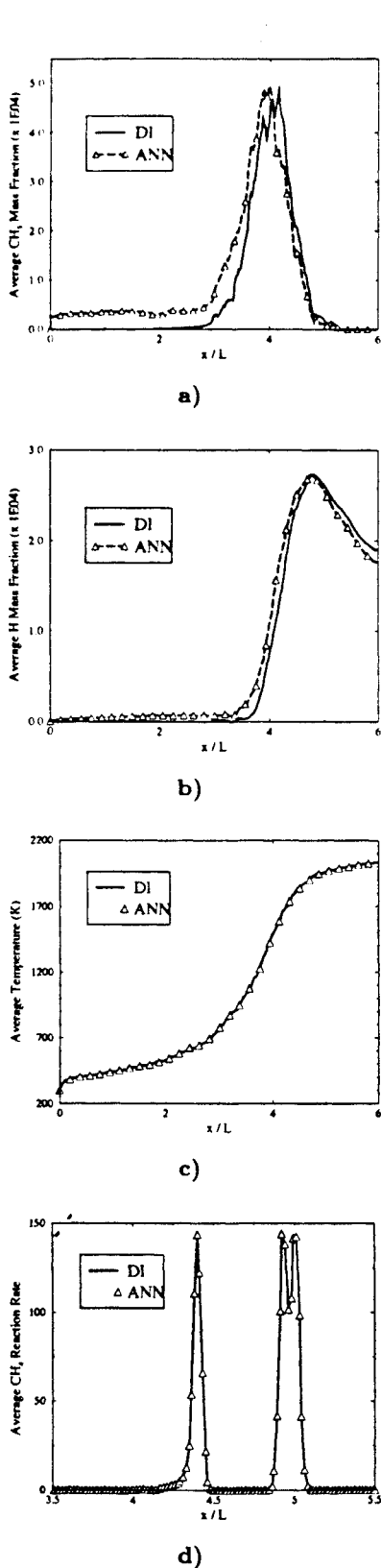**Fig. 6** Averaged profiles for product and pollutant species in the F1 flame).

6

a)

b)

c)

d)

Fig. 7 Averaged profiles for minor species, temperature and CH_4 reaction rate (F1 flame).
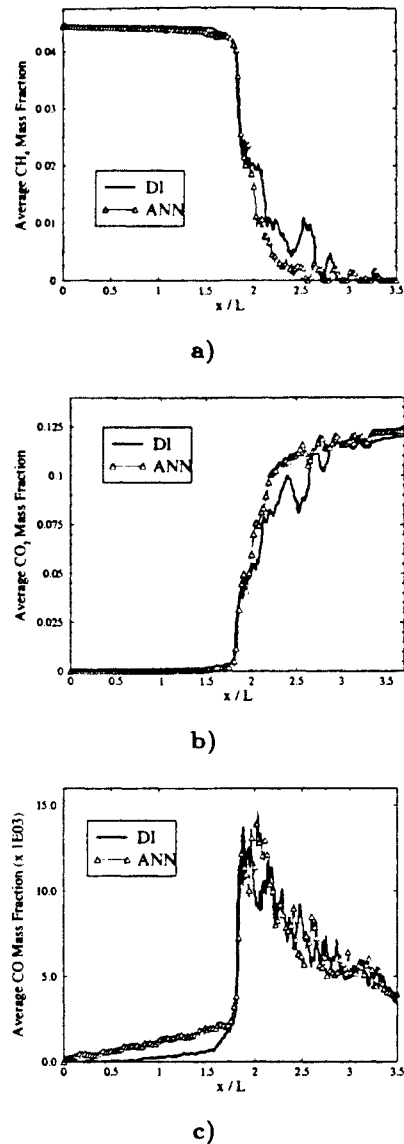

a)

b)

c)

Fig. 8 Average scalar profiles for some species (B1 flame).

ple to incorporate as compared to an ISAT algorithm, involving only a few matrix multiplications and additions and floating point operations. This can significantly reduce not only the memory overheads but also the overall cost of chemical composition update.

6 Conclusions

ISAT and ANN are both feasible and economical approaches for the simulation of scalar evolutions in a chemically reacting mixture. From a memory and storage point of view, ANN may offer a better alternative when implementing LES on massively parallel systems. The accuracy and ability of the network depends significantly on the choice of the ANN parameters used and the quality of the input-output sets used for the network training. The present predictions for the species and temperature variations using
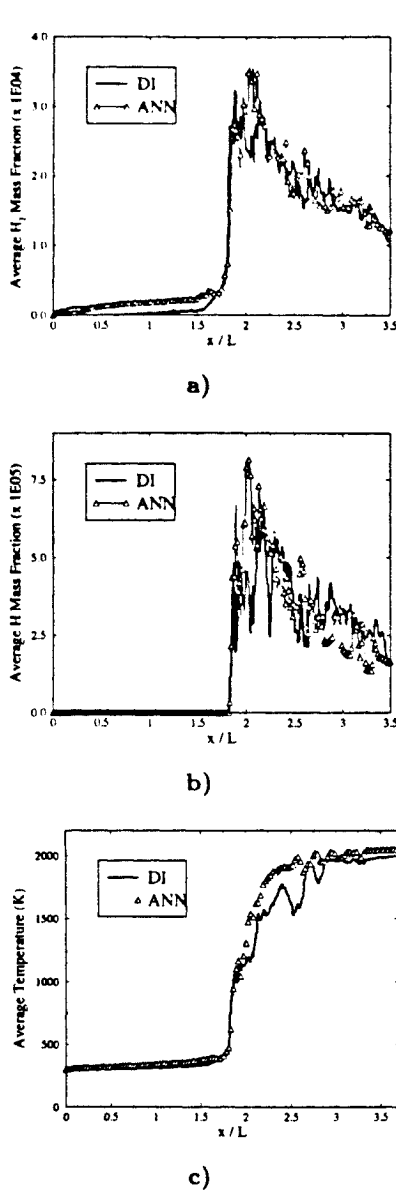
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a)

b)

c)

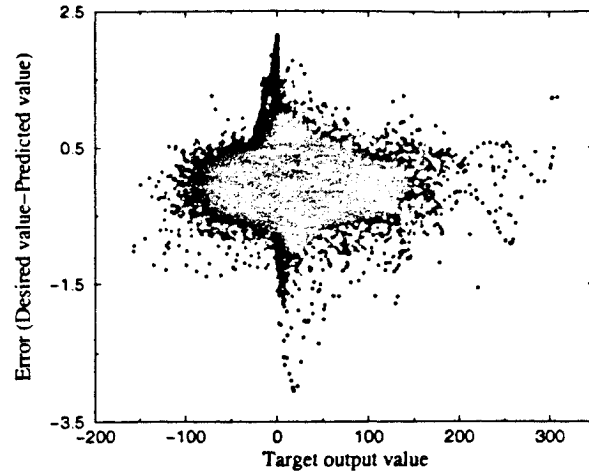**Fig. 9 Average scalar profiles for some species and temperature (B1 flame).**

Fig. 10 Network error obtained for one of the reactive scalars (H_2). x-axis denotes the actual target value, and y-axis shows the corresponding error in the ANN estimate.

tion of the turbulent reaction rates using a simple lookup model. Once this approach is validated it is likely to prove a major development for the implementation of turbulence-chemistry interactions in realistic combustors without requiring significant computational resources. Undoubtedly, this will involve more complicated ANNs than being used at present. However, preliminary studies show that this can be accomplished within the framework of the subgrid simulation model. The development and implementation of a "turbulent ANN" will be reported in the near future.

7 Acknowledgments

ANN compare well with those obtained with the conventional direct integration approach (using ISAT) for the two particular flame regimes considered. Currently work is underway to increase the accuracy of the neural nets obtained, for example, by choosing a better training sample set which can represent the accessed composition domain much better. Splitting the composition domains for each of the 20 ANNs on the basis of temperature or any other parameters, is also currently being studied, and will be reported in the future.

Finally, the next step in the modelling of turbulent combustion is the incorporation of the turbulence effects into the ANN structure, for example, the subgrid velocity scale and the range and sizes of the eddies. This will obviate the need to have an "on-line" LEM subgrid simulation model[4,6,7] and will allow predic-

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