GT-2002-30608

COMPUTATIONAL ISSUES FOR SIMULATING FINITE-RATE KINETICS IN LES

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Abstract

At present, large-eddy simulations (LES) of turbulent flames with multi-species finite-rate kinetics is computationally infeasible due to the enormous cost associated with computation of reaction kinetics in 3D flows. In a recent study, In-Situ Adaptive Tabulation (ISAT) and Artificial Neural Network (ANN) methodologies were developed for computing finite-rate kinetics in a cost effective manner. Although ISAT reduces the cost of direct integration considerably, the ISAT tables require significant on-line storage in memory and can continue to grow over multiple flow-through times (an essential feature in LES). Hence, direct use of ISAT in LES may not be practical, especially in parallel solvers. In this study, a storage-efficient Artificial Neural Network (ANN) is investigated for LES application. Preliminary studies using ANN to predict freely propagating turbulent premixed flames over a range of operational parameters are described and issues regarding the implementation of such ANNs for engineering LES are discussed.

1 INTRODUCTION

The potentially more stringent emission regulations that are expected in the near future have focused the need to develop more efficient, low-NO_x gas turbine systems. However, accurate prediction of mixing and combustion processes requires a comprehensive numerical model that can predict not only the flame structure and propagation characteristics but also is capable of predicting pollutant formation, and ignition/extinction phenomena. All these phenomena are unsteady features and therefore, steady state RANS methods cannot be employed. On the other hand, direct numerical simulations are not practical, since resolution and computational requirements far exceed even future computational capabilities.

Although LES has become popular in recent years to study unsteady turbulent processes, its use to predict reacting flows is still not well established. Since combustion process occurs at the small-scales, ad hoc models used at the resolved LES scale cannot provide an accurate estimation of the physical processes that are not even modeled. To address this limitation, recently, a method that combines conventional LES for the momentum transport with a subgrid reaction-diffusion simulation model was developed and demonstrated [1, 2]. In particular, the key feature of this subgrid model (called the linear-eddy mixing (LEM) model) is that both reaction kinetics and molecular diffusion processes are implemented within the subgrid domain as a direct simulation (and thus, requires no closure). In addition, since advection of the subgrid fields across LES cells is carried out using a Lagrangian transport model (see cited references) it allows both co- and counter-gradient diffusion processes to occur naturally at the resolved scales. This ability is particularly important in complex flows where large-scale coherent structures (that can cause counter-gradient diffusion) transport the chemical species into small-scale mixing regions (where gradient diffusion transport can dominate).

However, even in this approach, detailed reactions kinetics is computationally prohibitive for engineering level simulations. Simplifications based on the mixture fraction (for non-premixed) or the *G*-equation (for premixed) formulations (that have been employed in many recent studies), are limited by the inherent assumptions in these formulations. For example, mixture fraction formulation assumes equal diffusivity and a two-feed system. However, in a real gas turbine engine these assumptions are severe approximations since there are usually pilot and secondary flame zones resulting in the formation of multiple premixed, partially premixed and non-premixed zones. In premixed systems, although the *G*-equation approach can provide reliable prediction on flame-turbulence interactions and combustion dynamics, emission prediction is impossible since no chemical species are being tracked. Thus, LES of

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multi-species kinetics in realistic combustors will require a new approach that is not only computationally efficient but also accurate.

In recent studies, we have been focusing on issues regarding implementation of finite-rate kinetics within the subgrid reaction-diffusion model. Finite-rate chemistry (using a 19-species, 15-reaction methane-air mechanism) was recently implemented using ISAT to study freely propagating premixed flames in the thin-reaction-zone and wrinkled flamelet regimes [3] (see Fig. 1). In this study, the LEM model was implemented in a *stand-alone* mode to simulate the premixed flame. Results showed that the flames in these regimes can be predicted quite accurately using this model. However, in a parallel implementation, ISAT required significant memory storage (e.g., around 100+MB per processor) that quickly becomes a bottleneck. Therefore, recently [4], an alternate method based on ANN was investigated as a memory and cost-effective alternative to the ISAT model.

The use of ANN is widespread in the engineering community, but is relatively novel in combustion related CFD applications. Past studies [5, 6, 7, 8] have addressed the ability of ANN to accurately map the composition space. Recently [4], the ANN approach was used to simulate a turbulent premixed flame with a 19-species, 15-step methane-air mechanism [9]. In the present study, some new observations of this ANN model development are discussed along with a demonstration of how multiple ANNs for different flames can be combined to predict a new flame. The extension of this procedure for integration into LES model for engineering studies is also discussed.
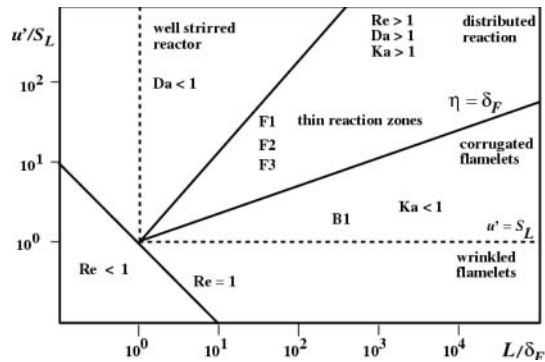

Figure 1. Diagram of turbulent premixed combustion regimes.

2 MODEL FORMULATION

The details of the LEM model have been given elsewhere [1, 3, 10, 11] and therefore, are only briefly summarized here. LEM is a stochastic model that treats reaction-diffusion and turbulent convection separately but concurrently. Reaction-diffusion processes evolve on a one-dimensional (1D) domain in which all the characteristic length scales in the turbulent field (from the integral scale L to the Kolmogorov η) are fully resolved (6 cells are used to resolve η). The orientation of the 1D domain is in the direction of the scalar gradient [10] (and thus, for premixed flame, is in the flame normal direction), and within this domain, the equations governing constant pressure, adiabatic flame propagation are

$$\frac{\partial Y_k}{\partial t} = -\frac{1}{\rho}\frac{\partial \rho Y_k V_k}{\partial x} + \frac{\dot{\omega}_k W_k}{\rho} + F_{kstir} \qquad (1)$$

$$\frac{\partial T}{\partial t} = -\frac{1}{\rho \overline{C_p}}\sum_{k=1}^{N} C_{p,k} Y_k V_k \frac{\partial T}{\partial x} + \frac{1}{\rho \overline{C_p}}\frac{\partial}{\partial x}(\overline{\kappa}\frac{\partial T}{\partial x}) - \frac{1}{\rho \overline{C_p}}\sum_{k=1}^{N} h_k \dot{\omega}_k W_k + F_{Tstir} \qquad (2)$$

The equation of state for the scalar mixture is $P = \rho T \sum_{k=1}^{N} \frac{Y_k R_u}{W_k}$ and the caloric relation is given by $h_k = \Delta h_{f,k}^0 + \int_{T0}^{T} C_{p,k}(T')dT'$. Here, T is the temperature, P is the thermodynamic pressure, R_u is the universal gas constant and ρ is the mass density. Also, $Y_k, W_k, C_{p,k}, \dot{\omega}_k, h_k, V_k$ and $\Delta h_{f,k}^0$ are respectively, mass fraction, molecular weight, specific heat at constant pressure, mass reaction rate, enthalpy, diffusion velocity and standard heat of formation (at standard temperature, T^o) of the k-th species. The mixture-averaged specific heat at constant pressure and thermal conductivity are respectively, $\overline{C_p}$ and $\overline{\kappa}$. The diffusion velocity is given by the Fick's law: $V_k = -\frac{D_k}{Y_k}\frac{dY_k}{dx}$, where D_k is the mixture-averaged diffusivity of the k-th species.

Since turbulent convection is implemented explicitly, the convective terms $u\partial Y_k/\partial x$ and $u\partial T/\partial x$ in the species and energy equations are symbolically represented as F_{kstir} and F_{Tstir}, respectively. These terms are implemented using stochastic re-arrangement events called triplet maps, each of which represents the action of a turbulent eddy on the scalar fields. It has been shown [10] that this mapping can capture correctly the physical increase in scalar gradient (without affecting the mean scalar concentration) due to eddy motion. Three parameters are needed to implement these turbulent stirring events: the typical eddy size l, the eddy location within the 1D domain and the stirring frequency (event rate) λ. The eddy size in the range L to η is determined randomly from an eddy size distribution $f(l)$ which is obtained using inertial range scaling in three-dimensional turbulence

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[10]: $f(l) = (5/3) l^{-8/3} / (\eta^{-5/3} - L^{-5/3})$. Here, η is determined from inertial range scaling law $\eta = N_\eta L Re^{-3/4}$ where N_η is an empirical constant. This constant reduces the effective range of scales between L and η but does not change the turbulent diffusivity, as described earlier [11].

The event location is randomly chosen from a uniform distribution and the event rate (frequency per unit length) is determined by [10]

$$\lambda = \frac{54}{5} \frac{\nu \, Re}{C_\lambda L^3} \frac{[(L/\eta)^{5/3} - 1]}{[1 - (\eta/L)^{4/3}]} \qquad (3)$$

The time interval between events is then given as $\Delta t_{stir} = 1/(\lambda X_{LEM})$ where X_{LEM} is the length of the 1D domain.

The unique feature of the LEM model is that although the scalar evolution is simulated in 1D, the effect of turbulence on the scalar fields is modeled using 3D scaling laws. As a result, flame wrinkling occurs at spatial and temporal scales that mimic effects of realistic 3D turbulent eddies on the laminar flamelets. The ability of LEM to capture realistic flames in the flamelet regime is now well documented [11].

The above formulation has two constants: C_λ and N_η both of which arise from the use of scaling laws. In the earlier studies [11], these parameters were obtained by comparing LEM predictions to experimental data [12] in the flamelet regime. The present study uses these same values ($C_\lambda = 15$ and $N_\eta = 4$) in order to determine if the LEM model validated in the flamelet regime can be applied to flames in the thin-reaction-zones regime without any adjustments.

The implementation of this LEM model within the LES framework has also been accomplished in recent years [1, 2]. In this approach, the LEM model is simulated locally within each LES cell to simulate the local reaction-diffusion and turbulent mixing processes, as noted in the cited literature.

3 NUMERICAL IMPLEMENTATION

Methane-air flames similar to those in the experiments are studied here. Two mechanisms, a one-step global mechanism (with five species) has been used to evaluate ANN integration issues and a more detailed 15-step, 19-species skeletal mechanism is employed for more realistic applications. This mechanism (which included NO_x kinetics) has been shown to be quite accurate over a wide range of equivalence ratios and is capable of predicting extinction and re-ignition.

The numerical method is the same as in the earlier study [3, 4] and therefore, only briefly summarized. To simulate a stationary flame, a moving observation window is used that translates with the flame brush to maintain approximately the same relative position between flame center and observation window (even though the flame propagates freely into the reactants). All statistics are obtained relative to the flame center. The computational domain is chosen large enough to fully capture this flame brush (typically $6L$). For this purpose a 1D domain length of 0.014355 m is chosen with 352 grid points.

Earlier studies [11] and the present study show that statistically, stationary flames can be simulated using this approach.

All spatial derivatives are computed using second-order accurate central scheme and a fractional operator splitting scheme is used to evolve the chemical state. The chemical source term is obtained either using ISAT or ANN depending upon the situation.

3.1 In-Situ Adaptive Tabulation

In ISAT, only the accessed region of the composition space which is a subset of the whole realizable region (i.e., the set of all possible combinations of compositions for a given number of species) is tabulated. This tabulation is done as a part of the simulation and when the same composition re-occurs, the table is searched and the stored information is retrieved using fast binary tree search algorithm. Since only the accessible region is stored, the overall time required to build, retrieve and store information reduces significantly. Further details of the ISAT algorithm is given elsewhere [13] and therefore, avoided here for brevity.

Here, a parallel (using MPI directives) implementation of LEM model (with ISAT) is used. Since, for the chemistry point problem no communication is needed, each processor builds a local table for the composition that occurs inside its domain. This localizes the ISAT table to each processor and reduces the overall load (including search and retrieve time) for each processor (as opposed to building a single table for all the composition that occurs over the whole of the domain).

Computational efficiency of ISAT is significant, as reported earlier [13]. The size of the table and cost depend upon the error tolerance (which determines the allowable error in each of the scalar for a given initial state). For higher accuracy, this parameter should be low, leading to an increase in the total simulation time and storage. In general, we have observed a speed-up of around 50 by using ISAT. This is consistent with the speedup reported earlier [13]. Additional speed up can be achieved by using a more extensive ISAT table setup.

3.2 Artificial Neural Network

An ANN structure consists of large interconnected non-linear processing elements, which

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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 data set 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.

Initially, 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. Each ANN is a three-layer scaled conjugate gradient (SCG) back-propagation network [14], 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 to be optimized iteratively. 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 dataset. However, it is still not clear if this is the optimal solution. On the other hand, use of the ISAT data reduces the cost of on-line evaluation of the chemical composition.

Subsequent analysis of the ANN predictions and comparison with ISAT predictions demonstrated that a single ANN for each species is not optimal to cover the entire operational regime. For example, it was observed that large changes occur within a small region, whereas there are locations ahead and behind the flame where very little changes are occurring. Furthermore, detailed analysis [4] showed that prediction of some of the key radicals (e.g. H, HO_2, etc.) using a single ANN for each species was

problematic. More recent ANNs employ 27 ANNs for *one* species (instead of 1 ANN) where the composition domain is (in term of the temperature field) subdivided into sub domains and ANNs trained on each of these sub domains.
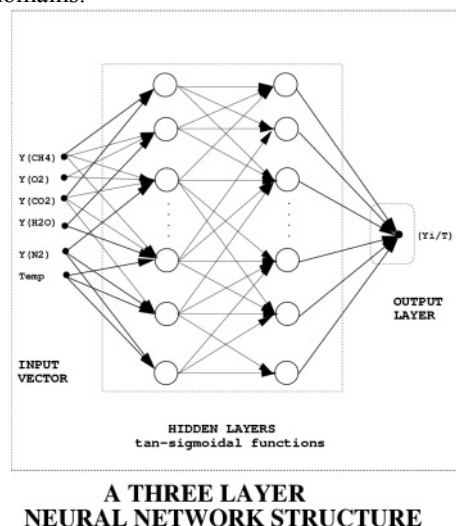

Figure 2. Artificial Neural Network trained on multi-species kinetics.

4 RESULTS AND DISCUSSION

The ANN structure is obtained after training is substituted for the calculation of the chemistry part. It is observed that the SCG training algorithm provides excellent agreement with the ISAT predictions. However, the key issue for LES is the incorporation of these off-line trained ANN into real flame simulations where other un-specified parameters/effects (e.g., flow, turbulent stirring, etc.) are also prevalent. We discuss this issue in the following discussion.

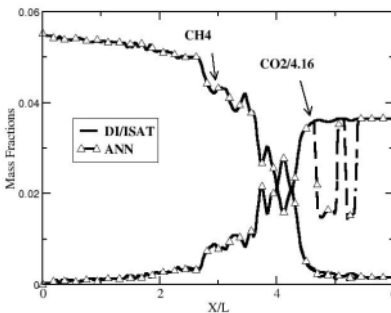### 4.1 Prediction of Turbulent Flames using Global Kinetics

To demonstrate the application of ANN to simulate a multiple of flames, the present effort has employed a one-step global mechanism [15] for 5 species (CH_4, O_2, N_2, CO_2 and H_2O). Two flames, Flames F1 and F3 are simulated using the same code and chemistry. Both these flames are in the thin-reaction-zone but encounter different turbulence intensity in the incoming flow. Two ANNs are trained independently on each of these flames and the ANN predictions are compared with ISAT (with Direct Integration when needed) prediction. Figures 3 and 4 show respectively, the instantaneous and time-averaged profiles of the key species and temperature for these flames. It can be seen that there is excellent agreement between the ISAT and ANN predictions (even in the instantaneous profiles).
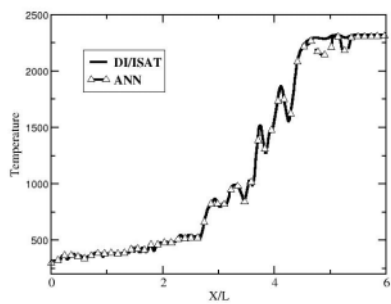
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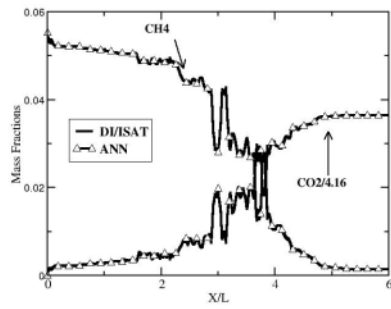
(a) F1 Flame
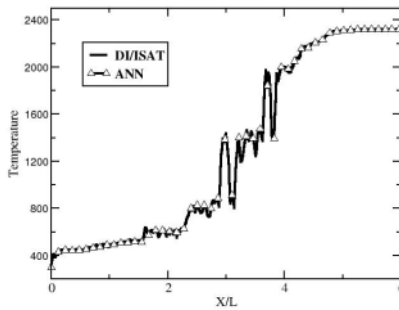
(a) F1 Flame

(b) F1 Flame

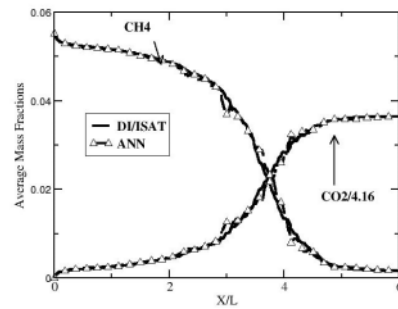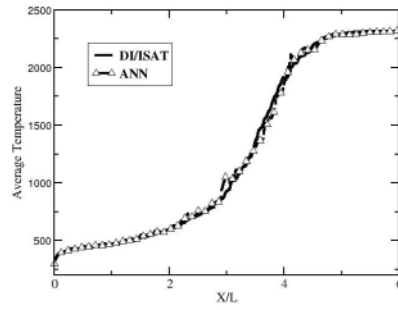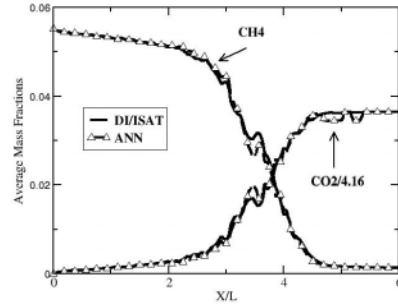(b) F1 Flame

(c) F3 Flame

(c) F3 Flame

(d) F3 Flame

Figure 3. Instantaneous profiles for the F1 and F3 flames.
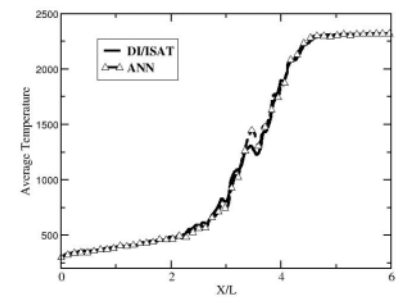
(d) F3 Flame

Figure 4. Time-averaged profiles for the F1 and F3 flames.

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Subsequent to these studies, another simulation was carried for conditions corresponding to the Flame F2 (see Fig. 1). This flame lies between the Flames F1 and F3. Instead of training a new ANN for this flame, the ANNs developed for Flames F1 and F3 were combined (i.e., a weighted interpolation of the prediction from F1 and F3 flames is used) to predict this new flame. Figure 5 shows that combining multiple ANNs to predict a new flame is possible. However, more development (some are noted below) is still needed before this methodology can be utilized for LES applications.

4.2 Prediction of Turbulent Flames using Detailed Kinetics

The 15-step, 19-species mechanism is also employed in some studies of these flames. Most of these results were reported earlier [4] and therefore, are only summarized here for completeness.

Figures 6 and 7 compare the ISAT and ANN predictions for some minor and pollutant species for the F1 flame. Clearly, the more complicated reaction mechanism can also be reasonably approximated using ANNs. There are, however, some key issues that have to be addressed in this case. In particular, the prediction of radicals that form in very low concentration in the flame zone is computationally very difficult and will require additional research. The impact of errors in key radicals on the pollutant formation also needs to be addressed. In particular, the use of multiple ANNs for each species (tailored based on their formation within the flame zone) is being evaluated to address this issue. Results from this study will be reported in the near future.

### 4.3 Application of ANN in Engineering LES

An extension of the LEM+ANN approach is also being developed to simulate turbulent flames within LES. In this approach, an additional ANN that contains turbulence parameters such as the subgrid intensity and range of turbulent eddies in the flame zone ($f(l)$) is being developed. For example, the F1-F3, and B1 flames all have different u' and $f(l)$. Therefore, by combining the thermo-chemical ANNs for these flames with the fluid mechanical ANN for u' and $f(l)$, it will be possible to directly obtain the filtered reaction rates. Here, we consider the filtered reaction rate as an average over all the turbulent eddies that have perturbed the chemical state. Thus, mathematically this can be written as: $\overline{\dot{\omega}}_m = <\dot{\omega}_m>$ where $\overline{\dot{\omega}}_m$ is the LES filtered reaction rate and $<\dot{\omega}_m>$ indicates the reaction rate averaged over the local eddies. The latter term can be approximated from the LEM approach as:
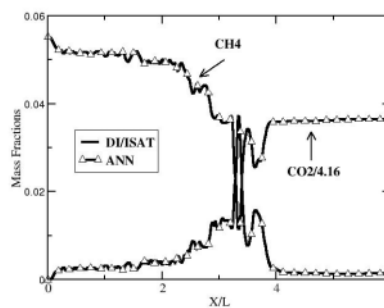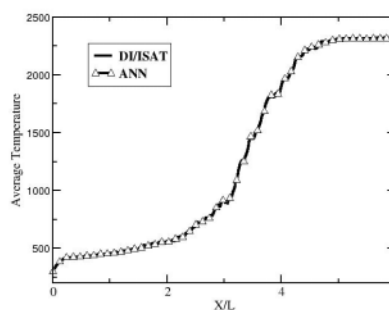

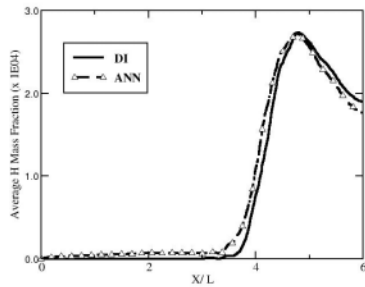(a) Instantaneous Profiles
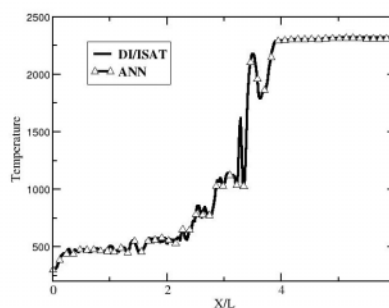
(b) Instantaneous Profiles
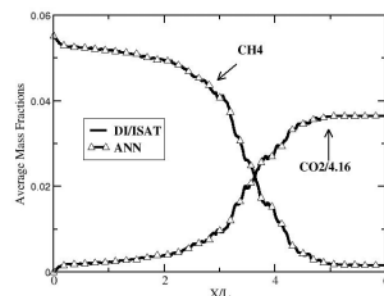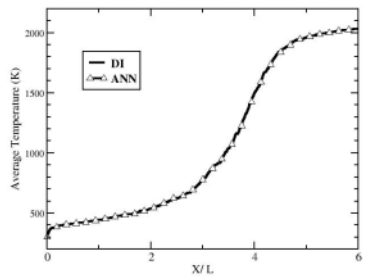

(c) Time-averaged Profiles

(d) Time-averaged Profiles
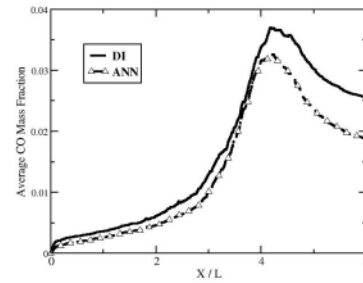Figure 5. Instantaneous and time-averaged profiles for F2 Flame
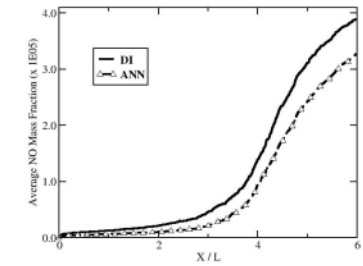
(a) *H* Profile

(a) *CO* Profile

(b) T Profile

Figure 6. Averaged profiles for minor specie H and temperature.

(b) *NO* Profile

Figure 7. Averaged profiles for pollutant species in the F1 Flame.

$< \dot{\omega}_m >= \int \dot{\omega}_m(l)f(l)d(l)$. This approach allows the inclusion of detailed kinetics into LES solvers without the associated (enormous) increase in computational effort since the term $< \dot{\omega}_m >$ can be determined and stored in the ANN. This approach is denoted Turbulent ANN (TANN) and is briefly described below.

To implement TANN, it is necessary to combine thermo-chemical and fluid-mechanical effects within a single formulation. To use it within the context of LEM, the F$_{stir}$ terms in Equations (1) and (2) are not implemented which means that the reaction diffusion equations are identical to the *laminar* case. In order to capture the effect of turbulent eddies on the flame, eddies are sampled from the eddy size pdf, *f(l)* at the local time scale (as before), and the eddy event rate and event location are determined as in the original LEM approach, except that, now the reaction rates in these eddy locations are implemented in an averaged sense. Figure 8 shows some preliminary results of the TANN prediction. The results when compared to the direct integration result show that there are regions where the local structure is getting smoothed by this averaging procedure. This is expected since in the TANN implementation, detailed

sub-structure of the flame (i.e., structure within eddies of size *l*) are not captured and only the integrated effect is included. In spite of some errors due to the implicit smoothing of the flame structure, the "filtered" profile shows the gradual temperature rise in the pre-heat zone (which is characteristic of a thin-reaction-zone flame). Further improvements of this TANN approach to obtain more accurate prediction are still underway.

Although the above study appears unrelated to LES, note that, we are attempting to estimate the "filtered" reaction rate by TANN. So far, only the eddy size distribution *f(l)* for a single flame F1 has been incorporated. However, once other relevant parameters, such as turbulence intensity *u'*, equivalence ratio, and inlet temperature are included (by using the LEM model simulations), TANN will essentially predict the filtered reaction rate as a function of these parameters. In other words, TANN will contain the joint pdf of thermo-chemical and fluid mechanical variables. To mathematically explain this approach, consider the filtered scalar equations that are typically solved in a conventional LES. [Note we are not considering the subgrid simulation model [2] here since this approach is considered too expensive for engineering-level LES.]:

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$$\frac{\partial \overline{\rho} \widetilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_i}[\overline{\rho} \widetilde{Y}_m \widetilde{u}_i - \overline{\rho} \overline{D}_m \frac{\partial \widetilde{Y}_m}{\partial x_i} + \Phi^{sgs}_{i,m} + \theta^{sgs}_{i,m}] = \overline{\dot{\omega}}_m$$

(4)

for m =1,N species. In this equation, the subgrid scalar flux, $\theta^{sgs}_{i,m} = \overline{\rho}[\widetilde{V_{i,m} Y_m} - \widetilde{V}_{i,m} \widetilde{Y}_m]$ and the filtered reaction rate term, $\overline{\dot{\omega}}_m$ require closure. In engineering LES, a gradient approximation: $\theta^{sgs}_{i,m} \approx -\frac{\overline{\rho} \nu_t \nabla \widetilde{Y}_m}{Sc_m}$, where Sc_m is a turbulent Schmidt number (assumed to be unity), can be employed for the subgrid scalar flux. This approach is acceptable since the large-scale motion is resolved in the LES, and therefore, any large-scale counter-gradient processes (if they occur) are resolved (even when a gradient closure is employed for $\theta^{sgs}_{i,m}$).

The closure for $\overline{\dot{\omega}}_m$ is the key problem in LES. For example, the most popular approach is the assumed pdf approach in the mixture fraction space but this approach is not considered appropriate when complex kinetics and pollutant formation have to be predicted. The subgrid LEM model [1, 2] avoids this assumed pdf approach by simulating the actual local evolution of the joint-scalar pdf and therefore, provides an elegant closure for the scalar field. However, this approach is too expensive for engineering application. In the new TANN approach, the joint pdf for the thermo-chemical and fluid mechanical processes will be stored and accessed on-line to directly obtain $\overline{\dot{\omega}}_m$. As noted earlier, this results in $< \dot{\omega}_m >$ which is stored in the TANN.

There is another subtle advantage of TANN. Since it is built using Equations (1) and (2), it contains within it molecular diffusion (and differential diffusion) process (the term $\Phi^{sgs}_{i,m}$ in the above equation). Since molecular process occurs in the small-scales, it cannot (and should not) be modeled at the LES scale. The TANN data base contains within it molecular diffusion (in effect simulates $\Phi^{sgs}_{i,m}$ and therefore, does not have to be modeled. Furthermore, the diffusion term in the above equation, $\overline{\rho} \overline{D}_m \frac{\partial \widetilde{Y}_m}{\partial x_i}$ is a special term in the TANN approach since it incorporates diffusion across LES cell faces only under special circumstances (e.g., molecular diffusion when there is no flow). However, in high-Re turbulent flows

(where $\theta^{sgs}_{i,m}$ is likely to dominate at the resolved scales), this term could be neglected.

Further development of TANN is still underway in order to make this approach robust and applicable to a wide range of problems within the LES context. An approach we are now exploring is to implement the subgrid LEM model within each LES cell as a surrogate to obtain information on the eddies and their consequence on stirring. In this approach, the scalar fields are still solved on the LES grid (as done for the earlier TANN) but the subgrid field is interrogated between each LES time-step to determine how many eddies from the distribution *f(l)* contribute to turbulent mixing. The chemical ANN is then evolved within each local eddy of size *l* in-between the LES time-step and the final states are ensemble-averaged to obtain $< \dot{\omega}_m >$ in *each* LES cell. This filtered reaction rate term carries the subgrid scale information of turbulent stirring and reaction, to the coarser LES grid. Since the frequency and number of stirrings are still decided based on the 3D scaling laws of LEM, this approach will capture the effects of turbulent mixing on the filtered reaction rate without significantly increasing the computational cost. This approach combines the strengths of TANN and on-line LEM and may be general enough for wide applications. We hope to report on these studies very soon.

4.4 Computational Cost of TANN in a LES

The primary reason to use TANN is to reduce the computational cost (memory and runtime). As our recent studies have shown, ANN drastically reduces the memory requirement by an order of magnitude or more [4]. For example, a 150 MB ISAT table for 19-species mechanism reduces to less than 2 MB for ANN. Also, the computation time for ANN retrievals can be orders of magnitude less than that for ISAT, especially for more complicated mechanisms, like the 15-step, 19-species mechanism discussed before. Furthermore, since the ANN can be built using different time-interval beforehand, the cost for direct integration is completely eliminated. It is expected that once the TANN approach has been fully developed and integrated into a LES methodology, an engineering level LES with detailed kinetics will become feasible since the cost of obtaining the filtered reaction rate has been reduced to just the TANN access cost.

5 CONCLUSIONS

ISAT and ANN are both feasible and economical approaches for the simulation of scalar evolutions in a chemically reacting mixture. From memory and storage point of view, ANN may be a better alternative when implementing LES on

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massively parallel PC clusters. 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 ANN compare well with those obtained with ISAT for the various flames considered.
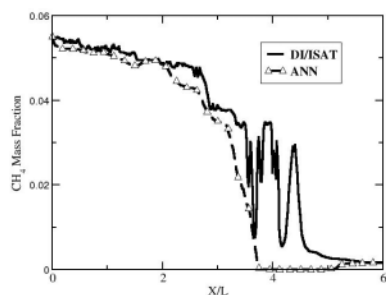
(a) CH_4 Profile
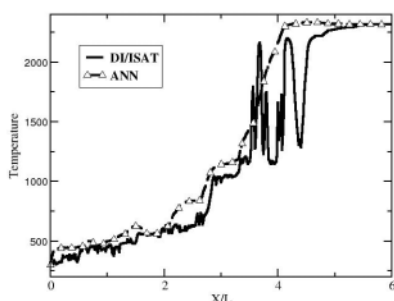
(b) T Profile

Figure 8. Instantaneous profiles for F1 flame using TANN

The next step is to implement the TANN approach in a LES model. This will obviate the need to have an "on-line" LEM simulation model and will allow prediction of the turbulent reaction rates using a simple lookup model. Some preliminary results are reported here using this new TANN approach. Once this approach is fully validated it is likely to prove a major development for reacting flow LES studies. Undoubtedly, this will involve more complicated ANNs than being used at present. However, preliminary studies show that this can be accomplished.

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