

**LARGE EDDY SIMULATION OF SYNGAS-AIR  
DIFFUSION FLAMES WITH ARTIFICIAL NEURAL  
NETWORKS BASED CHEMICAL KINETICS**

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# NOMENCLATURE

## Abbreviations

*AGDR* Adaptive Gradient Descent Rule

*AN* Artificial Neuron

*ANN* Artificial Neural Network

*CMC* Conditional Moment Closure

*DI* Direct Integration

*DI – LEMLES* DI used to compute the laminar source term in the LEM subgrid combustion model within the LES framework

*DNS* Direct Numerical Simulation

*GDR* Gradient Descent rule

*LANN* Laminar (instantaneous) Artificial Neural Network

*LANN – LEMLES* LANN used to compute the laminar source term in the LEM subgrid combustion model within the LES framework

*LDKM* Localized Dynamic  $k$ -equation Model

*LEM* Linear Eddy Mixing

*LEMLES* LEM used as a subgrid combustion model within the LES framework

*LES* Large Eddy Simulation

*MMC* Multiple Mapping Conditioning

*PDF* Probability Distribution Function

$PE$  Processing Element

$TANN$  Turbulent (filtered) Artificial Neural Network

$TANN - LES$  TANN used to compute the filtered source term directly within the LES framework

## Subscripts

$LEM$  quantity related to LEM scale

## Greek Symbols

$\alpha$  thermal diffusivity or the global momentum coefficient for ANN

$\chi$  scalar dissipation rate based on mixture fraction

$\chi_{st}$  scalar dissipation rate on stoichiometric plane

$\Delta_t$  time step size

$\delta_{ij}$  Kronecker delta

$\delta_m[k]$  local error term of Processing Element  $m$  at  $k$ -th iteration

$\Delta_{diff}$  diffusion time step size

$\Delta_{stir}$  stirring time step size

$\dot{\omega}_i$  chemical reaction rate of the  $i$ -th species

$\epsilon$  rate of dissipation of turbulent kinetic energy

$\eta_k$  pure viscosity of the  $k$ -th species

$\eta$  Kolmogorov length scale or the global learning coefficient in ANN

$\kappa$  thermal conductivity

$\lambda_k$	pure conductivity of the $k$ -th species
$\lambda$	stirring frequency
$\mu$	mixture viscosity
$\nu_t$	turbulent viscosity
$\Omega^{(1,1)}$	correction factor
$\bar{\Delta}$	large eddy simulation grid cut-off scale
$\phi_{ij}[k]$	gradient of training error w.r.t. weight coefficient joining AN pair $i$ and $j$
$\rho$	density
$\rho_t$	density at time instant $t$
$\tau_{ij}$	viscous stress tensor
$D_k^T$	thermal diffusion coefficient of the $k$ -th species
$D_{jk}$	binary diffusion coefficient of the species $i$ and $j$
$k_B$	Boltzman constant
$\omega_T$	heat release rate due to combustion

### **Others**

$\hat{\phantom{x}}$	test filter
$\tilde{\phantom{x}}$	Favre spatial filter
-	space average

### **Roman Symbols**

$(D_k)_m$	mixture averaged diffusion coefficient of the $k$ -th species
-----------	---------------------------------------------------------------

$b_i$	bias value of Artificial Neuron $i$
$C_\nu$	model coefficient for turbulent viscosity
$C_\epsilon$	model coefficient for subgrid dissipation
$c_{p,k}$	specific heat at constant pressure per unit mass of the $k$ -th species
$D^{sgs}$	dissipation of subgrid turbulent kinetic energy
$D_i$	molecular diffusivity of the $i$ -th species
$d_i$	desired output for the Artificial Neural Network training
$Da$	Damkohler number
$E$	total energy
$e$	internal energy
$E[k]$	Artificial Neural Network training error at the $k$ -th iteration
$F_{k, stir}$	turbulent stirring for $k$ -th species in LEM species equation
$F_{T, stir}$	turbulent stirring for temperature in LEM energy equation
$h_k$	species enthalpy per unit mass of $k$ -th species
$J_{i,k}$	diffusion flux of the $k$ -th species in the $i$ -th direction
$k^{sgs}$	subgrid turbulent kinetic energy
$l$	integral length scale
$L_{ij}$	Leonard's stress
$m_{ij}$	reduced molecular mass of the species pair $i$ and $j$
$N_s$	number of species

$net_i$	input signal received by $i$ -th Artificial Neuron
$p$	pressure
$P^{sgs}$	production of subgrid turbulent kinetic energy
$Pr$	Prandtl number
$q_i$	heat flux in the $i$ -th direction
$R_u$	universal gas constant
$Re$	Reynold's number
$Re_\Delta$	subgrid Reynold's number
$S$	strain rate
$Sc_t$	turbulent Schmidt number
$T$	temperature
$t$	time
$u'$	<i>rms</i> velocity
$u_i$	velocity in $i$ -th direction
$V_i^C$	correction velocity in the $i$ -th direction
$V_{i,k}$	diffusion velocity of the $k$ -th species in the $i$ -th direction
$W_k$	molecular weight of the $k$ -th species
$W_{ji}$	strength of weight connection between Artificial Neuron pair $i$ and $j$
$x_i$	Cartesian coordinate in $i$ -th direction
$X_k$	mole fraction of the $k$ -th species

$Y_k^{t+\Delta t}$  mass fraction of  $k$ -th species at time instant  $t + \Delta t$

$Y_k^t$  mass fraction of  $k$ -th species at time instant  $t$

$Y_i$  mass fraction of the  $i$ -th species

$y_n$  output of the  $n$ -th Artificial Neuron

$Z$  mixture fraction

$g()$  activation function used by an Artificial Neuron

### **Superscripts**

$R$  resolved subgrid fluctuation

$S$  unresolved subgrid fluctuation

$sgs$  subgrid scale

$'' , '$  fluctuating quantity

## SUMMARY

In the present study syngas-air diffusion flames are simulated using LES with artificial neural network (ANN) based chemical kinetics modelling and the results are compared with previous direct numerical simulation (DNS) study [14], with the objective of obtaining speed-up in chemistry computation while still having the accuracy of a stiff ODE solver. The DNS test case exhibits significant extinction-reignition and forms a challenging problem for ANN. The ANN methodology is used in two ways: 1) to compute the instantaneous source term in the linear eddy mixing (LEM) subgrid combustion model used within LES framework, i.e., laminar-ANN used within LEM-LES framework (LANN-LEMLES, hereafter), 2) to compute the filtered source terms directly within the LES framework, i.e., turbulent-ANN used within LES (TANN-LES, hereafter), which further increases the computational speed. A thermo-chemical database is generated from a standalone one-dimensional LEM simulation and used to train the LANN for species source terms on grid-size of Kolmogorov scale [34]. To train the TANN coefficients the thermo-chemical database from the standalone LEM simulation is filtered over the LES grid-size and then used for training [32]. To evaluate the performance of the TANN methodology, the low  $Re$  test case is simulated with direct integration used for chemical kinetics modelling in LEM subgrid combustion model within the LES framework (DI-LEMLES, hereafter), LANN-LEMLES and TANN-LES. The TANN is generated for a low range of  $Re_t$  in order to simulate the specific test case. The conditional statistics and pdfs of key scalars and the temporal evolution of the temperature and scalar dissipation rates are compared with the data extracted from DNS. Results show that the TANN-LES methodology can capture the extinction-reignition physics with reasonable accuracy compared to the DNS. Another

TANN is generated for a high range of  $Re_t$  expected to simulate test cases with different  $Re$  and a range of grid resolutions. The flame structure and the scalar dissipation rate statistics are analysed to investigate success of the same TANN in simulating a range of test cases. Results show that the TANN-LES using TANN generated for a large range of  $Re_t$  is capable of capturing the extinction-reignition physics with a very little loss of accuracy compared to the TANN-LES using TANN generated for the specific test case. The speed-up obtained by TANN-LES is significant compared to DI-LEMLES and LANN-LEMLES.



# CHAPTER I

## INTRODUCTION

In non-premixed flames the heat release rate is controlled by the molecular mixing rate of fuel and oxidizer, which is a process occurring at small scales and hence, the combustion process essentially takes place at small scales. However, the large scale convection process due to turbulence enhances the rate of fuel-oxidizer mixing by straining and affects the combustion process. The rate of fuel-oxidizer mixing is characterized by scalar dissipation rate [29] which is a function of molecular diffusivity  $D$  and gradient of mixture fraction  $Z$  [1]. Initially as  $\chi$  increases the rate of molecular mixing increases and the rate of burning also increases. However, if  $\chi$  exceeds a critical value (extinction scalar dissipation rate,  $\chi_q$ ) over prolonged periods of time, then the diffusive heat loss becomes greater than the rate of heat release due to chemical reactions leading to temperature drop and reactants leaking through the reaction zone resulting in local extinction. The mixing process continues during this period and local packets of partially premixed and non-premixed mixtures are formed. This mixture can either reignite on its own once  $\chi$  reduces or by coming close to burning regions in the surroundings. Understanding the extinction-reignition phenomenon is important because modern combustion systems require efficient mixing for enhanced burning which is obtained by increasing  $\chi$ . However, large values of  $\chi$  leads to extinction-reignition process which destabilizes the flame and also increases emissions due to incomplete combustion [29].

## 1.1 *Flame-Turbulence Interaction*

Previous direct numerical simulation (DNS) studies [36, 37, 14, 27] have investigated the extinction-reignition process in turbulent non-premixed flames. Sripakagorn et al. [36, 37] in their studies of non-premixed combustion in decaying isotropic turbulence using one-step global reaction, observed that the average scalar dissipation rate at stoichiometric mixture fraction ( $\chi_{st}$ ) remained lower than the extinction scalar dissipation rate even though the fluctuations of the instantaneous  $\chi_{st}$  showed large values over  $\chi_q$  causing local extinction events. They observed that reignition occurs due to three reasons: 1) once the  $\chi_{st}$  drops the flamelet reignites on its own (independent flamelet scenario), 2) edge flame propagation, 3) a hot neighbourhood engulfs the unburnt packet. Besides, the probability of reignition is highest due to independent flamelet scenario. Pantano et al.[27] in their studies of methane-air diffusion flames showed that higher order reaction mechanisms are needed for detailed investigation of extinction-reignition phenomenon. Hawkes et al.[14] studied temporally evolving syngas-air diffusion flames with significant extinction-reignition. They used an 11 species, 21 steps skeletal reaction mechanism to study the evolution of flame structure and the characteristic of mixture fraction  $Z$  and showed that the predictions with the skeletal mechanism is in good agreement with the detailed mechanism.

Modelling the spatially filtered chemical source terms and the turbulence-chemistry interaction forms a challenging problem in LES since combustion process is a small scale process [29, 28]. DesJaridin et al. [10] showed that modelling the reaction term by directly using the filtered resolved scales in the chemical kinetics model gives poor agreement when compared with DNS results. This is observed when chemical reaction rates are comparable with the rate of mixing, i.e., the turbulence-chemistry interaction is strong and hence the subgrid fluctuations of the scalar field can no longer be neglected.

Various closure models have been studied in the past. Joint PDF methods provide

exact closure to the source terms, but increase in the number of species increases the dimensionality of the joint PDF and makes it expensive. Besides, the molecular diffusion terms are unclosed and the quality of the predictions depend on the applied mixing model and the values of the constants used [39]. Multiple mapping conditioning (MMC) is a cheaper option which reduces the dimensions of the reference space depending on the problem and captures extinction-reignition with reasonable accuracy. However, choosing the reference space is a challenging task. Cleary et al. [9] in their studies of turbulent non-premixed flames showing extinction-reignition used a single mixture-fraction-like variable and up to three dissipation like variables. Results showed poor accuracy of the model in case of moderate extinction-reignition, even though it predicted significant extinction-reignition and global extinction with reasonable accuracy. First order flamelet model and conditional moment closure (CMC) model singly conditioned on mixture-fraction with first moment closure reduces the dimensionality to one but breaks down when extinction-reignition phenomenon are present [29],[23]. Because in singly conditioned CMC model with first order closure approximation only the average  $\chi_{st}$  appears and the fluctuations of  $\chi_{st}$  are neglected. Hence close to extinction-reignition where the fluctuations of  $\chi_{st}$  are large the model breaks down. CMC closure based on a precomputed parameterized reference field that maps reactive species mass fractions as functions of mixture fraction and sensible enthalpy have successfully captured the extinction-reignition phenomenon [24]. However, this requires the reference field to be continuously adjusted during computation, to ensure consistency with the CMC solution and doubly conditioned chemical source terms that are functions of time, space, mixture fraction, and sensible enthalpy can thus be obtained.

The flamelet model assumes the PDF of mixture fraction and scalar dissipation rate at stoichiometric mixture fraction ( $\chi_{st}$ ) as marginal beta and log-normal distributions, respectively, which do not hold good near extinction-reignition scenarios where there

are high levels of chemical non-equilibrium [13]. Pitsch et al. [30] studied the influence of stochastic fluctuations of the scalar dissipation rate on the solution of the flamelet equations and suggested a new transport term in the flamelet equations modelled by a stochastic mixing approach and an additional stochastic differential equation for the scalar dissipation rate. Second order CMC models have shown improvement in capturing extinction-reignition phenomenon in hydrocarbon jet diffusion flames using detailed kinetics[20]. However, additional equations for the conditional variances and covariances of each pairing of reactive species are required, which makes CMC expensive for detailed reaction mechanisms. Besides, the second order correlations need to be determined from DNS data. First order CMC model doubly conditioned on mixture fraction and scalar dissipation rate is another alternative; however, it predicts the onset of reignition too early [4].

Linear eddy mixing (LEM) model used as a subgrid combustion model within LES framework (LEMLES) closes the reaction-diffusion equation in an exact sense and captures extinction-reignition with accuracy [32]. However, using LEM model with the stiff ODE solver to find source terms is computationally expensive.

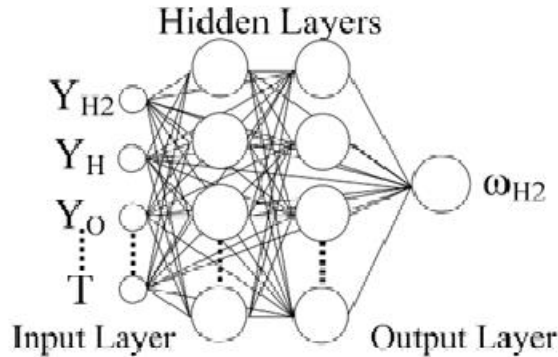
To reduce the cost of chemical kinetics evaluation in LEMLES, Sen et al. [32] used an artificial neural networks (ANN) based chemical kinetics modelling, which eliminates the stiff ODE solver to calculate the subgrid laminar reaction rates (LANN).

## ***1.2 Artificial Neural Networks (ANN)***

Artificial neural networks are modelled after the biological neurons [25]. The ANN is made of a number of simple highly interconnected processing elements (PEs) which process information by its dynamic state response to external inputs. It is an interpolation scheme. Contrary to the conventional approach of solving equations, ANN learns by example and provides predictions into new states. An ANN architecture is as shown in Fig. 1. The large circles are the Processing Elements (PEs) and the lines

joining them are the weight connectors. The first layer of PEs from left is the input layer, the middle two layers of PEs are the hidden layers, and the fourth layer is the output layer. The set of input/output pairs of PEs are representative of the physical process. The purpose of the hidden layers is to make the ANN capable of modelling complex data. Choosing the correct number of processing elements in a hidden layer is another challenging task. If an inadequate number of processing elements are used in a hidden layer, the net will not be able to model complex data. On the other hand, if too many neurons are used, training time will become excessively long and the model may memorize the data. This result in ANN net fitting the data for which is trained extremely well but generalizing poorly to new unseen data. In the given example, the N number of inputs, which include mass fraction of all the species and temperature, are used to compute the species reaction rate of  $H_2$ , by interpolation.

Fig.2 show two AN pairs. Each connection between a particular AN (Artificial



**Figure 1:** Representation of an Artificial Neural Network Architecture

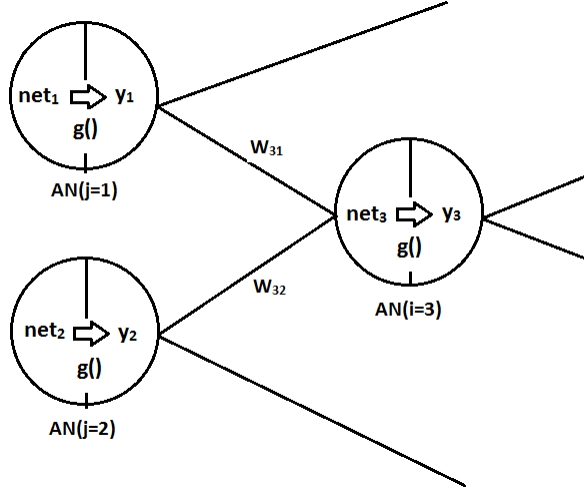
Neuron) pair ( $i$  and  $j$ ) has a weight coefficient  $W_{ji}$ , which defines the strength of the connection between the AN pair. The combined effect of all ANs connected to  $AN_i$ , acting as an input vector for  $AN_i$  is:

$$net_i = \sum_{j=0}^J W_{ij} [k] y_j - b_i \quad (1)$$

where  $y_j$  is the signal fired from  $AN_j$  to  $AN_i$  and  $W_{ij}$  is the respective weight coefficient and  $b_i$  represents the internal threshold for the  $AN_i$ . The net output of  $AN_i$  is:

$$y_i = g(\text{net}_i) \quad (2)$$

where  $g$  is an activation function. For a given ANN architecture and input/output



**Figure 2:** Description of Artificial Neuron pairs

pairs, the weight coefficients are determined through a training process. The objective is to train long enough such that the ANN predicts well for both train and test data, while not so long that the ANN memorizes the train data, giving very good predictions for train data and poor predictions for test data. Hence, it is important to stop the training at the correct time because long training times may again lead to memorization of data. In the present study if the training error does not reduce for 100 consecutive sweeps of the training table, the training is stopped and the weight coefficients calculated before last 100 sweeps are used in the ANN.

Past studies have successfully used ANN for function approximation, classification, time series prediction, data association, optimization in a variety of applications such as, electro magnetics [7], forecasting [40], land cover classification and mapping [8] and chemical kinetics modelling with significant memory savings and speed-up. Christo

et al. [6] used artificial neural networks (ANN) model based chemical kinetics for a systematically reduced  $\text{H}_2\text{-CO}_2$  system, consisting of three steps and four controlling scalars. The ANN was implemented with transported-PDF (Monte Carlo) approach. Blasco et al. [2] in addition to simulating the species evolution, used ANN for providing the density and temperature. Ihme et al. [16] proposed a generalized method for the generation of optimal artificial neural networks. They tested it with the methane-hydrogen/air flame in a bluff-body swirl-stabilized burner configuration using LES to investigate the effect of long-time error accumulation in the statistical data during the simulation[17]. However all these studies generated the training table for ANN by either three-dimensional simulations of cases similar to the actual test case or randomly generating compositions within allowable compositional bounds. These compositional bounds have to be selected carefully for an efficient ANN and are specific to a problem. Further, the random selection of training samples lead to bias of the training set towards the steady state situation and a better selection criteria based on the degree of chemical activity of a state had to be used.

Sen et al. [34] generated the training table for ANN by using off-line (standalone 1D) LEM computations. This table did not require any compositional bounds and did not show any bias towards steady state. The ANN was trained using this table. The ANN generated was used in the LEMLES simulation to compute the laminar reaction rates. Hence, ANN was generated without a-priori knowledge of the actual thermochemical data space of test case. To further reduce the cost of computation, Sen [35] used the off-line LEM computations, but instead of tabulating the laminar reaction rates, the filtered reaction rates representative of the LES were tabulated along with the filtered thermochemical data [35]. Hence, the trained ANN (TANN) directly estimated the filtered reaction rates within the LES framework and eliminated the need of LEM with significant cost reduction. In the current effort, the TANN approach is further analysed, to investigate the development of a general TANN to simulate a

range of cases with varying Reynolds number and grid resolutions. Further, the key parameters affecting the development of the general TANN is analysed.

### **1.3 Objectives**

Syngas or synthetic gas mixtures can be produced from a wide variety of sources including coal, biomass, organic waste, and refinery residuals. It consists of mainly  $CO$  and  $H_2$  in various proportions. When derived from biomass and other industrial waste it forms a cheap and renewable source of energy. Because of the large coal resources available worldwide, there is strong interest in coal-based integrated gasification combined cycle power generation. Hence, understanding the behaviour of syngas is very crucial for its industrial usage. This thesis studies the extinction-reignition phenomenon in temporally evolving syngas-air flames using ANN for chemical kinetics modelling. Test cases are chosen from a previous direct numerical (DNS) study of temporally evolving syngas-air diffusion flames with 21 steps, 11 species reduced chemical kinetics[14]. These cases exhibit complex extinction-reignition phenomenon for a range of flow Reynolds number and varying levels of turbulence. The degree of extinction also increases with increase in  $Re$  which leads to lower mean temperature and longer re-ignition times. Hence, these cases form a challenging problem for the development of a general TANN. The main objective is to obtain considerable speed-up while having the same accuracy as DI. The objectives in details are as follows:

- Study extinction-reignition in non-premixed flames using ANN for laminar (instantaneous) reaction rates (LANN) with LEMLES framework.

To evaluate the accuracy and speed-up of the ANN methodology, it is used to simulate a temporally evolving jet flame for a low Reynolds number case. A



DNS study is selected as the test case from literature [14]. The thermochemical database for training ANN is generated using a one-dimensional standalone LEM computation, instead of using actual LES simulation data. The standalone LEM covers a wide range of flame-turbulence interaction. It is expected that it will cover a large thermo-chemical data space and the thermochemical data space of the LES simulation will form just a subset of the LEM thermochemical data space. Hence, the ANN for computing the instantaneous reaction rates can be generated without a-priori knowledge of the LES thermochemical data space. The instantaneous reaction rate is obtained as a function of temperature and species concentration.

$$\frac{\dot{\omega}_i}{\rho} = f(Y_1, \dots, Y_{N_s}, T) \text{ where, } i=1, \dots, N_s \quad (3)$$

For a given pressure and LEM time step size ( $\Delta t$ )

The source terms in the subgrid combustion model within the LEMLES simulation is computed using ANN. The conditional PDFs of the species extracted from the LANN-LEMLES and compared with the DI-LEMLES and DNS study to evaluate the accuracy of the LANN generated. The evolution of the scalar-dissipation PDFs during extinction and reignition are also investigated.

- Study extinction-reignition in non-premixed flames using ANN for filtered reaction rates (TANN).

To further increase, the speed-up of the LES simulation, ANN is trained to calculate the filtered reaction rates directly within the LES framework. Using the standalone LEM, the filtered reaction rates are tabulated by applying a spatial filter on the 1D LEM domain data. The filtered reaction rate is trained in the ANN as a function of filtered mass fractions, temperature, subgrid Reynolds number, and filtered level species gradient. A fixed filter size representative of the LES grid size is used for spatial filtering. The filtered source term is trained

as a function of the subgrid Re and filtered species gradient to take into account the effect of turbulence.

$$\frac{\bar{\omega}_i}{\bar{\rho}} = f \left( \tilde{Y}_1, \dots, \tilde{Y}_{N_s}, \tilde{T}, Re_{\Delta}, \frac{\partial \tilde{Y}_i}{\partial x_j} \right) \text{ where, } i=1, \dots, N_s \quad (4)$$

For a given pressure, filter size and LES time step size ( $\Delta t$ )

The TANN is used to calculate the filtered reaction rates in the LES simulation of the temporally evolving syngas-air jet flames and the results are compared with the DNS study to evaluate the accuracy of TANN.

- Study extinction-reignition in non-premixed flames using a single TANN for a range of cases.

The TANN approach is explored further and a generalized TANN net is developed by training it over data collected from standalone LEM simulation run over a large range of  $Re_t$ . This TANN net is used to simulate a range of cases with varying Reynolds number and grid resolutions. The success of a generalized TANN net for a range of cases will lead to significant time savings. Otherwise, every new a case will require generation of a new TANN which will consume time and resources.

- Study extinction-reignition using TANN trained as a function of species scalar dissipation rate.

The filtered reaction rate is obtained from the ANN as a function of filtered mass fractions, temperature, subgrid Reynolds number and filtered level species dissipation rate. The use of filtered level species dissipation rate instead of species gradient is more relevant to modelling filtered species reaction rate, because lighter species have higher molecular diffusivity D, and for for the same species gradient dissipate much faster than the heavier species and affect the

filtered source term largely.

$$\frac{\bar{\omega}_i}{\bar{\rho}} = f \left( \tilde{Y}_1, \dots, \tilde{Y}_{N_s}, \tilde{T}, Re_\Delta, 2D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \cdot \frac{\partial \tilde{Y}_i}{\partial x_j} \right) \text{ where, } i = 1, \dots, N_s \quad (5)$$

The results obtained are compared with the DNS study and TANN-LES trained as a function of species gradient instead of species scalar dissipation rate.

## CHAPTER II

### COMPUTATIONAL MODELLING

In the present chapter, first the general Navier-Stokes equations are described. Second the stand-alone LEM modelling is described. The stand-alone LEM simulation is used to generate the thermochemical data for training the ANN without a-priori knowledge of the actual 3D simulation. Third the tabulation method for TANN is described. Fourth, ANN architecture and its training is described. Finally the LES modelling and subgrid combustion modelling is explained.

#### *2.1 Gas Phase Governing Equations*

The gas phase governing equations of continuity, momentum, energy and species in the conserved form, in the absence of external forces, MHD effects, etc, are given as:

$$\begin{aligned}
 \frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} &= 0 \\
 \frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} [\rho u_i u_j + p \delta_{ij} - \tau_{ij}] &= 0 \\
 \frac{\partial \rho E}{\partial t} + \frac{\partial}{\partial x_i} [(\rho E + p) u_i - u_j \tau_{ji} + q_i] &= 0 \\
 \frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i} [\rho Y_k u_i + J_{i,k}] &= \dot{\omega}_k
 \end{aligned} \tag{6}$$

where,  $k = 1, \dots, N_s$

In the above equations  $\rho$  is the density,  $u_i$  is the  $i$ -th velocity component,  $E$  is the total energy,  $Y_k$  is the  $k$ -th species mass fraction and  $N_s$  represents the total number of species in the flow.  $\tau_{ij}$  is the viscous stress tensor and is computed as:

$$\tau_{ij} = \mu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \mu \frac{\partial u_k}{\partial x_k} \tag{7}$$

where  $\delta_{ij}$  is the Kronecker function ( $\delta_{ij} = 1$  if  $i = j$ ;  $\delta_{ij} = 0$  if otherwise), and  $\mu$  is the dynamic viscosity. The total energy  $E$  is the sum of internal energy ( $e$ ) and kinetic

energy, is given as:

$$E = e + \frac{1}{2}u_k u_k \quad (8)$$

In this formulation the internal energy per unit mass is:

$$e = \sum_{k=1}^{N_s} Y_k h_k - \frac{p}{\rho} \quad (9)$$

The  $k$ -th species total enthalpy is calculated as the sum of the chemical and sensible enthalpies as:

$$h_k(T) = \Delta h_{h,k}^0 + \int_{T_0}^T c_{P,K}(T') dT' \quad (10)$$

In the above equation  $\Delta h_{h,k}^0$  is the enthalpy of formation at the reference temperature and pressure  $T_0, P_0$ . The second represents sensible enthalpy, which is a function of temperature and  $c_{P,k}$  is the heat capacity at constant pressure for the  $k$ -th species.

The pressure in equation (6) is derived from the perfect gas equation of state:

$$p = \rho R_u T \sum_{k=1}^{N_s} \frac{Y_k}{W_k} \quad (11)$$

where,  $R_u, N_s, W_k$  are the universal gas constant, number of species and molecular weight of  $k$ -th species, respectively.

The mass reaction rate per unit mass ( $\dot{\omega}_k$ ) for the  $k$ -th species is calculated by solving the ODE representing a given reaction mechanism. For the given initial concentration of the species and a time step size, the ODE solver is used to find the new scalar field at the end of the time step. The reaction rate is calculated as:

$$\dot{\omega}_k = \frac{(Y_k^{t+\Delta t} - Y_k^t)\rho^t}{\Delta t} \quad (12)$$

The heat flux ( $q_i$ ) and the  $k$ -th species diffusion flux ( $J_{i,k}$ ) introduced in Eq. (6) are defined as:

$$q_i = \sum_{k=1}^{N_s} J_{i,k} h_k - \kappa \nabla T - \sum_{k=1}^{N_s} \frac{R_u T}{W_k X_k} D^T d_{ik} \quad (13)$$

$$J_{i,k} = \rho Y_k V_{i,k} \quad (14)$$

The last term in Eq.(13) is neglected in the present simulation where  $D_K^T$  is the thermal diffusion coefficient.  $V_{i,k}$  is the  $k$ -th species diffusion velocity. The species diffusion velocity takes into account mass diffusion caused by concentration gradients (ordinary diffusion), temperature gradients (Soret effect) and pressure gradients. In the present study the effect of pressure gradients and temperature gradients is neglected. Mixture-averaged formulation is used to find the diffusion velocity instead of more accurate multi-component formulation, because the latter approximation requires inverting an  $N_s \times N_s$  matrix to find the multi-component diffusion coefficients. The diffusion velocity for a mixture averaged formulation is given as:

$$V_{i,k} = -\frac{1}{X_k} (D_k)_m \frac{\partial X_k}{\partial x_i} \quad (15)$$

where the mixture diffusion coefficient for the  $k$ -th species is:

$$(D_k)_m = \frac{\sum_{j \neq k}^{N_s} X_j W_j}{W_m \sum_{j \neq k}^{N_s} X_j / D_{jk}} \quad (16)$$

where  $D_{jk}$ 's are the binary diffusion coefficients. It assumes a two component binary mixture, where species  $j$  is diffusing into species  $k$ . Based on kinetic theory of gases, the binary diffusion coefficients are calculated as:

$$D_{jk} = \frac{3}{16} \frac{\sqrt{2\pi k_B^3 T^3 / m_{jk}}}{p\pi\sigma_{jk}^2 \Omega^{(1,1)}} \quad (17)$$

where  $k_B$  is the Boltzman constant,  $\sigma_{jk}$  is the mean diameter ( $= (\sigma_{jk} + \sigma_{jk})/2$ ), and  $\Omega^{(1,1)}$  is the correction factor used to modify the ideal gas law to account for the molecular interactions. The reduced mass  $m_{jk}$  is the given by:

$$m_{jk} = \frac{m_j m_k}{m_j + m_k} \quad (18)$$

The mixture averaged formulation needs to satisfy the net species diffusion flux to zero ( $\sum_{k=1}^{N_s} V_{i,k} Y_k = 0$ ) for conservation of mass. This is done by adding a correction velocity to the convective terms in the species conservation equation to account for

the excess diffusion. The correction velocity is calculated as:

$$V_i^C = - \sum_{k=1}^{N_s} Y_k \left( \frac{1}{X_k} (D_k)_m \frac{\partial X_k}{\partial x_i} \right) \quad (19)$$

With the correction the  $k$ -th species diffusion flux is calculated as:

$$J_{i,k} = \rho Y_k (V_{i,k} + V_i^C) \quad (20)$$

The mixture averaged viscosity given by Vilke's formula:

$$\mu = \sum_{k=1}^{N_s} \frac{X_k \eta_k}{\sum_{k=1}^{N_s} X_k \Phi_{kj}} \quad (21)$$

where

$$\Phi_{kj} = \frac{1}{\sqrt{8}} \left( 1 + \frac{W_k}{W_j} \right)^{-\frac{1}{2}} \left( 1 + \left( \frac{\eta_k}{\eta_j} \right)^{\frac{1}{2}} \left( \frac{W_j}{W_k} \right)^{\frac{1}{4}} \right)^2 \quad (22)$$

where  $\eta_i$  is the  $i$ -th species viscosity. The thermal conductivity is calculated in a similar manner using the following formula:

$$\kappa = \frac{1}{2} \left( \sum_{k=1}^{N_s} X_k \lambda_k + \frac{1}{\sum_{k=1}^{N_s} X_k / \lambda_k} \right) \quad (23)$$

where  $\lambda_k$  is the pure species conductivity.

## 2.2 Stand-alone LEM

Off-line stand-alone LEM computations are performed to evaluate the scalar field evolution due to the turbulence-chemistry interaction. The following reaction-diffusion equations are solved along a 1D grid initialized with a laminar diffusion flame:

$$\begin{aligned} \rho \frac{\partial Y_k}{\partial t} &= F_{k, stir} - \frac{\partial}{\partial s} (\rho Y_k V_{k,s} + \rho Y_k V_s^C) + \dot{\omega}_k \\ \rho C_p \frac{\partial T}{\partial t} &= F_{T, stir} - \rho \frac{\partial T}{\partial s} \left( \sum_{k=1}^{N_s} C_{p,k} Y_k (V_{k,s} + V_s^C) \right) + \frac{\partial}{\partial s} \left( \kappa \frac{\partial T}{\partial s} \right) + \dot{\omega}_T \end{aligned} \quad (24)$$

In Eq.24 the  $\dot{\omega}_k$  represents the reaction rate and  $\dot{\omega}_T = - \sum_{k=1}^{N_s} h_k \dot{\omega}_k W_k$  represents the heat release due to combustion, where  $W_k$  denotes the molecular weight of the  $k$ -th species. The reaction rates are obtained by direct integration of the chemical kinetics

model.  $V_{k,s} = -D_{k,m}(W_k/WY_K)(\partial X_k/\partial s)$  is the diffusion velocity of the  $k$ -th species, diffusivity of the  $k$ -th species in the mixture is  $D_{k,m} = \left(\sum_{j \neq k}^{N_s} X_j W_k\right) / W \sum_{j \neq k}^{N_s} X_j / D_{j,k}$ , where  $W$  represents the mixture molecular weight and  $D_{j,k}$  represents the binary diffusion coefficient and  $V_s^C$  is the velocity correction to ensure mass conservation[31]. Turbulent advection is symbolically represented by  $F_{k,stir}$  and  $F_{T,stir}$  and modelled as numerical re-arrangement events (triplet-maps)[18]. The assumption behind the stirring model is that, the turbulent advection stochastically re-distributes the concentration gradients, without changing the scalar values and increases the scalar gradients and the molecular diffusion competes with it by smoothing them out. The reaction-diffusion equation proceeds at a time step size determined as  $\Delta t_{diff} = 0.25(\Delta s)^2 / \max(D_k, \alpha)$ . Turbulent stirrings proceed at its own time-scale given by  $\Delta t_{stir} = 1/(\lambda L)$ , where  $\Delta s, \alpha, L, \lambda$  denote the LEM grid resolution, thermal diffusivity, LEM domain length and stirring frequency, respectively.

### ***2.3 Tabulation method for TANN and training***

The LEM simulation is initialized with a laminar profile obtained for a given thermochemical composition and the turbulence-chemistry interaction is simulated for a given range of  $Re_t$ . For LANN, the training database was constructed by tabulating the instantaneous composition and temperature from the LEM domain at regular intervals of time along with the laminar reaction rates obtained by directly integrating the chemical kinetics [34],[33]. The tabulation strategy for TANN differs slightly. The results here are filtered by a spatial filter size representative of the LES grid resolution. Fig. 3 shows the variation of the mixture fraction along the 1D LEM domain at a given instant of time. Larger gradients are observed at the LEM level, whereas a smoother profile is observed at the LES level because the spatial filtering process smoothens the effect of large gradients at small scales on an average sense.



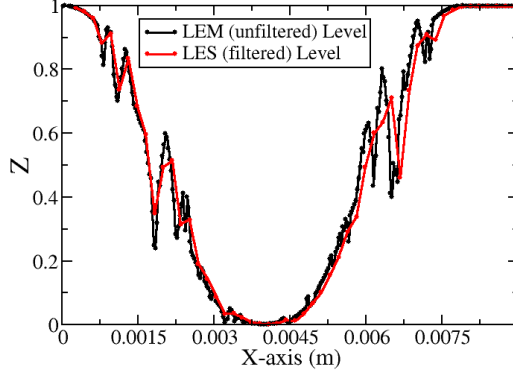
In the earlier study [34], the laminar reaction rate was parametrized with respect to the instantaneous species mass fractions and temperature:

$$\frac{\dot{\omega}_i}{\rho} = f(Y_k, T) \quad (25)$$

However, the filtered reaction rates are functions of the LES filter size and turbulence, in addition to the filtered mass fractions and temperature. Hence, filtered reaction rates are parametrized as:

$$\frac{\bar{\omega}_i}{\bar{\rho}} = f\left(\tilde{Y}_k, \tilde{T}, Re_\Delta, \frac{\partial \tilde{Y}_i}{\partial x}\right) \quad (26)$$

where,  $\tilde{Y}_k, T$  and  $\frac{\partial \tilde{Y}_i}{\partial x}$  represent the filtered species mass fractions, filtered temperature and filtered species gradient.  $Re_\Delta$  denotes the sub grid Reynolds number in the LES framework and is calculated as  $Re_\Delta = u'\Delta/\nu$ , where  $u' = \sqrt{(2/3)k^{sgs}}$  and  $\Delta$  is the LES grid filter. In the stand-alone LEM simulation, based on the  $Re_t$  and  $l_0$  (integral length scale) the other parameters like grid spacing, stirring length and stirring frequency are selected [18]. However,  $Re_t$  is a global variable for the stand-alone LEM and it differs from local variable  $Re_\Delta$  in the LES. Stand-alone LEM provides the scalar field evolution and does not provide any information about the local turbulence levels. To calculate  $Re_\Delta$  the values of kinetic energy  $k$  and  $u'$  are initially set equal to zero in the LEM domain. Then as the simulation proceeds and turbulent stirrings take place,  $u'$  is updated by value  $\frac{\nu Re_t}{\eta}$  during a stirring event at the grid locations where it occurs. The turbulence is assumed to be homogeneous and  $u'$  in all the three directions is assumed equal, which is consistent with LEM assumption based on universal nature of small scales. The effect of dissipation is



**Figure 3:** Variation of mixture fraction ( $Z$ ) along the 1D standalone LEM domain at the DNS level and the LES level

taken into account and the value of  $u'$  is updated as follows:

$$\begin{aligned}
 k &= \frac{3}{2}u'^2 \\
 \epsilon &= \frac{k^{1.5}}{\Delta s} \\
 k &= \text{Max}((k - (\epsilon * \Delta t_{diff})), 0) \\
 u' &= \sqrt{(2/3)k}
 \end{aligned} \tag{27}$$

The  $Re_{\Delta}$  is calculated as a function of the  $u'$  (obtained from Eq. 27),  $\nu$  averaged over the filtered grid size and the filtered grid size.

The TANN table generated is used to train a given ANN architecture. Finally, the TANN chemical kinetics model is used within the LES framework to calculate the filtered reaction rates (TANN-LES).

## 2.4 Artificial Neural Networks

An acyclic ANN architecture is used in the present study with a predefined number of hidden layers and processing elements [35, 34]. The ANN code based on back-propagation learning with gradient descent rule is used in the present study. The

training algorithm consists of two parts: a) forward propagation of the input, b) backward propagation of the error. The output of a processing element  $i$  at iteration  $k$  is given as:

$$y_i[k] = g(\text{net}_i[k]) \quad (28)$$

where

$$g(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}} \quad (29)$$

where  $g()$  is the hyperbolic tangent activation function.  $\text{net}_i$  in Eq. 28 represents the effect of all PEs connected to the PE  $i$ .  $\text{net}_i$  is calculated as:

$$\text{net}_i[k] = \sum_{m=0}^M W_{im}[k]y_m[k] - b_i[k] \quad (30)$$

where,  $W_{im}[k]$  is the weight coefficient between PEs  $i$  and  $m$ ,  $y_m[k]$  is the output of the PE  $m$ ,  $b_i[k]$  is the internal threshold for the PE  $i$  and  $M$  is the number of PEs connected to the PE  $i$ . After calculating the output for all PEs, the global error  $E[K]$  defined as the difference between the desired ( $d_i$ ) and the calculated ( $y_i[k]$ ) value at the output layer, for the current weight distribution, is calculated:

$$E[k] = \frac{1}{2} \sum_{i=1}^I [d_i - y_i[k]]^2 \quad (31)$$

where  $I$  denotes the PE in the output layer. This error is back propagated to all the PEs and the new weight coefficients are calculated using GDR. Weights of the connections are adjusted according to the gradient of the local error across each connection:

$$W_{ij}[k+1] = W_{ij}[k] - \eta \frac{dE[k]}{dW_{ij}[k]} \quad (32)$$

where  $\eta$  is the global learning coefficient which is constant and same for all PEs and iterations. The idea behind the gradient descent rule is to find a particular weight distribution which provides the minimum global error. Eq. 32 calculates the gradient of the error with respect to the individual weights. The gradient of the error with

respect to the weight coefficient for a connection between the output and a hidden layer is:

$$\frac{dE[k]}{dW_{ij}[k]} = - [d_i - y_i[k]] g' (net_i[k]) y_i[k] \quad (33)$$

for rest of the connections it is calculated as:

$$\frac{dE[k]}{dW_{ij}[k]} = - \left[ \sum_{m=1}^M \delta_m[k] W_{mi}[k] \right] g' (net_i[k]) y_j[k] \quad (34)$$

here  $\delta_m[k]$  is the local error term of the PE  $m$ . Its value depending on if the PE  $m$  is at the output or a hidden layers is given as:

$$\delta_m[k] = \begin{cases} [d_m - y_m[k]] g' (net_m[k]) & \text{if output layer} \\ g' (net_m[k]) \cdot \sum_{z=0}^Z W_{zm}[k] \delta_z[k] & \text{if hidden layers} \end{cases} \quad (35)$$

The error surface may have local minima and a momentum coefficient ( $\alpha$ ) is used to find the global minimum. The eq. 32 is modified as:

$$\Delta W_{ij}[k] = -\eta \Delta E[k] + \alpha \Delta W_{ij}[k - 1] \quad (36)$$

The momentum coefficient ( $\alpha$ ) like the learning rate coefficient ( $\eta$ ) is also the same for all the PEs and constant for all iterations.

The determination of the proper values of the model coefficients ( $\eta, \alpha$ ) is a major challenge of the standard GDR. A large  $\alpha$  causes the algorithm to diverge and a same  $\eta$  cannot be used in the valleys or shallow regions of the error surface topology. An AGDR approach for self determining the model coefficients with respect to the error surface topology is used in the present work [35]. This method is based on the fact that all PEs have their own model parameters ( $\eta_{ij}$  and  $\alpha_{ij}$ ) and they are updated at every ANN iterations. The model coefficients are updated as:

$$\begin{aligned} \eta_{ij}[k + 1] &= \eta_{ij}[k] + \Delta \eta_{ij}[k] \\ \alpha_{ij}[k + 1] &= \alpha_{ij}[k] + \Delta \alpha_{ij}[k] \end{aligned} \quad (37)$$

where  $\Delta\eta_{ij}[k]$  and  $\Delta\alpha_{ij}[k]$  are calculated as:

$$\Delta\eta_{ij}[k] = \begin{cases} \kappa_1\lambda\eta_{ij} & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] > 0 \\ -\kappa_1\lambda\eta_{ij} & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] < 0 \\ 0 & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] = 0 \end{cases}$$

$$\Delta\alpha_{ij}[k] = \begin{cases} \kappa_1\lambda\alpha_{ij} & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] > 0 \\ -\kappa_1\lambda\alpha_{ij} & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] < 0 \\ 0 & \text{if } \phi_{ij}[k]\bar{\phi}_{ij}[k-1] = 0 \end{cases} \quad (38)$$

where  $\lambda = (1 - \exp(-\kappa_2\phi_{ij}[k]))$ ,  $\phi_{ij}[k] = \frac{\partial E}{\partial W_{ij}}$  and  $\bar{\phi}_{ij}[k] = (1 - \theta)\phi_{ij}[k-1] + \theta\phi_{ij}[k]$ . Here  $\kappa_1$  and  $\kappa_2$  are the second order model coefficients selected to be 0.1 and 0.01, respectively.

## 2.5 LES Modelling

LES approach is employed to solve the fully compressible, reacting, multi-species, Favre averaged form of the conservation equations. The LES equations are obtained by spatially filtering the Navier-Stokes equations, in order to separate the large geometry dependent scale structures from the small-scale structures which are considered universal. In LES the large scales are fully resolved where as the small scales (subgrid-scales) are modeled by using subgrid momentum and combustion models. In the current study, a spatial top hat Favre filter is applied to the Navier Stokes equations, with a kernel size equal to the grid spacing ( $\Delta x$ ), and the Favre-filtered LES equations are obtained with all subgrid unclosed terms explicitly identified. This filtering operation decomposes the flow variable ( $f$ ) into resolved Favre filtered ( $\tilde{f}$ ) and unresolved subgrid ( $f''$ ) components. The Favre-filtered variable  $\tilde{f}$  is defined by:

$$\tilde{f} = \frac{\overline{\rho f}}{\bar{\rho}} \quad (39)$$

$$f = \tilde{f} + f'' \quad (40)$$

where  $\rho$  is the local fluid density.

The following Favre-filtered form of the Navier Stokes equations are solved in the

current study:

$$\begin{aligned}
\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i}{\partial x_i} &= 0 \\
\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} [\bar{\rho} \tilde{u}_i \tilde{u}_j + \bar{p} \delta_{ij} - \bar{\tau}_{ij} + \tau_{ij}^{sgs}] &= 0 \\
\frac{\partial \bar{\rho} \tilde{E}}{\partial t} + \frac{\partial}{\partial x_i} [(\bar{\rho} \tilde{E} + \bar{p}) \tilde{u}_i + \bar{q}_i - \tilde{u}_j \bar{\tau}_{ji} + H_i^{sgs} + \sigma_i^{sgs}] &= 0 \\
\frac{\partial \bar{\rho} \tilde{Y}_k}{\partial t} + \frac{\partial}{\partial x_i} [\bar{\rho} \tilde{Y}_k \tilde{u}_i + \bar{\rho} \tilde{Y}_k \tilde{V}_{i,k} + \phi_{i,k}^{sgs} + \theta_{i,k}^{sgs}] &= \bar{\omega}_k
\end{aligned} \tag{41}$$

In Eq.(41) the total energy  $E$  is defined as the sum of kinetic energy and internal energy, the Favre averaged total energy  $\tilde{E}$  is given by:

$$\tilde{E} = \tilde{e} + \frac{1}{2} \widetilde{u_k u_k} \tag{42}$$

$$= \tilde{e} + \frac{1}{2} \tilde{u}_k \tilde{u}_k + \frac{1}{2} (\widetilde{u_k u_k} - \tilde{u}_k \tilde{u}_k) \tag{43}$$

$$= \tilde{e} + \frac{1}{2} \tilde{u}_k \tilde{u}_k + k^{sgs} \tag{44}$$

where  $\tilde{e}$  is the filtered internal energy and  $k^{sgs}$  is the unresolved or subgrid part of the kinetic energy. The filtered pressure is calculated as the filtered equation of state as[11]:

$$\bar{p} = \overline{\rho R T} = \bar{\rho} \widetilde{R T} \tag{45}$$

$$= \bar{\rho} \widetilde{R T} + \bar{\rho} R_u T^{sgs} \tag{46}$$

where  $R$  is the mixture gas constant. In the current study  $T^{sgs}$  is neglected.  $\tilde{V}_{i,k}$  is filtered diffusion velocity of the  $k$ -th species and is given as:

$$\tilde{V}_{i,k} = -\frac{\bar{D}_{km}}{\tilde{X}_k} \frac{\partial \tilde{X}_k}{\partial x_i} + \widetilde{V}_i^C \tag{47}$$

where  $\bar{D}_{km}$  is the mixture averaged species diffusivity and  $\widetilde{V}_i^C$  is the correction velocity. The filtered heat flux vector is given by:

$$\bar{q}_i = -\bar{\kappa} \frac{\partial \tilde{T}}{\partial x_i} + \bar{\rho} \sum_{k=1}^{N_s} \tilde{h}_k \tilde{Y}_k \tilde{V}_{i,k} + \sum_{k=1}^{N_s} q_i^{sgs} \tag{48}$$

where  $\tilde{h}_k$  and  $\bar{\kappa}$  denote the Favre filtered  $k$ -th species enthalpy and thermal conductivity. All the subgrid-scale terms are denoted with  $sgs$  are unclosed and they need to be modeled. These terms are the subgrid shear stress ( $\tau_{ij}^{sgs}$ ), subgrid viscous work ( $H_i^{sgs}$ ), subgrid viscous stress ( $\sigma_i^{sgs}$ ), subgrid mass flux ( $\phi_{i,k}^{sgs}$ ), subgrid diffusive mass flux ( $\theta_{i,k}^{sgs}$ ), and subgrid heat transfer via turbulent convection of species ( $q_{i,k}^{sgs}$ ). The subgrid terms in details are represented as:

$$\begin{aligned}
\tau_{ij}^{sgs} &= \bar{\rho} (\widetilde{u_i u_j} - \tilde{u}_i \tilde{u}_j) \\
H_i^{sgs} &= \bar{\rho} (\widetilde{E u_i} - \tilde{E} \tilde{u}_i) + (\overline{p u_i} - \tilde{p} \tilde{u}_i) \\
\sigma_i^{sgs} &= (\overline{u_j \tau_{ij}} - \tilde{u}_j \tilde{\tau}_{ij}) \\
\phi_{i,k}^{sgs} &= \bar{\rho} (\widetilde{Y_k u_i} - \tilde{Y}_k \tilde{u}_i) \\
\theta_{i,k}^{sgs} &= \bar{\rho} (\widetilde{V_{i,k} Y_k} - \tilde{V}_{i,k} \tilde{Y}_k) \\
q_{i,k}^{sgs} &= \bar{\rho} (\widetilde{h_k Y_k V_{i,k}} - \tilde{h}_k \tilde{Y}_k \tilde{V}_{i,k})
\end{aligned} \tag{49}$$

The closure strategy to model the subgrid terms is presented in the next sections.

### 2.5.1 Subgrid Momentum Modeling

An eddy viscosity type closure is adopted for momentum and energy transport because the major effect of small scales is to provide dissipation to the energy budget of the flow. the eddy viscosity,  $\nu_t$ , is evaluated using a characteristic length-scale, provided by the local grid size  $\bar{\Delta}$  where  $\bar{\Delta} = (\Delta_x \Delta_y \Delta_z)^{\frac{1}{3}}$ , and a subgrid velocity, obtained from the subgrid kinetic energy  $k^{sgs}$ , so that  $\nu_t = C_\nu \bar{\Delta} \sqrt{k^{sgs}}$ . The subgrid momentum tensor is modeled as:

$$\tau_{ij}^{sgs} = -2\bar{\rho}\nu_t \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{k,k} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij} \tag{50}$$

where  $Pr_t$  is the turbulent Prandtl number ( $Pr_t = 0.6$ )[3]. The two unclosed terms in the energy equation,  $H_i^{sgs}$  and  $\sigma_i^{sgs}$  are modeled together as:

$$H_i^{sgs} + \sigma_i^{sgs} = -2\bar{\rho} \frac{\nu_t}{Pr_t} C_p \frac{\partial \tilde{T}}{\partial \tilde{x}_i} + \tau_{i,j}^{sgs} \tilde{u}_i - \left( \rho \frac{\nu_t}{Pr_t} + \mu \right) \frac{\partial \tilde{k}^{sgs}}{\partial x_i} \tag{51}$$

For closure an additional transport equation for the subgrid scale kinetic energy  $k^{sgs}$  is solved, which is in the form of:

$$\frac{\partial \bar{\rho} k^{sgs}}{\partial t} + \frac{\partial}{\partial x_i} (\bar{\rho} \tilde{u}_i k^{sgs}) = P^{sgs} - D^{sgs} + \frac{\partial}{\partial x_i} \left( \frac{\bar{\rho} \nu_t}{Pr_t} \frac{\partial k^{sgs}}{\partial x_i} \right) \quad (52)$$

where  $P^{sgs} = -\tau_{ij}^{sgs} \frac{\partial \tilde{u}_i}{\partial x_j}$ , and  $D^{sgs} = C_\epsilon \bar{\rho} \left( \tilde{k}^{sgs} \right)^{\frac{3}{2}} / \bar{\Delta}$ , are the production and the dissipation of the  $k^{sgs}$ , respectively. In this equation,  $Pr_t = 1$ , the two coefficients,  $C_\nu$  and  $C_\epsilon$  have constant value of 0.067 and 0.916, based on earlier calculations. The present study uses a dynamic approach (LDKM hereafter) to compute the model coefficients  $C_\nu$  and  $C_\epsilon$ , based on the assumption that the resolved and the unresolved small scales behave in a similar manner and hence the model coefficients can be computed from similarity relations[21, 22]. Based on experimental observations it was found that for high Reynolds number flows the subgrid stress ( $\tau_{ij}^{sgs}$ ) at the grid filter level  $\bar{\Delta}$  and the Leonard's stress ( $L_{ij}$ ) at the test filter level ( $\hat{\Delta} = 2\bar{\Delta}$ ) are self-similar.  $L_{ij}$  is given by the following expression:

$$L_{ij} = \langle \bar{\rho} \tilde{u}_i \tilde{u}_j \rangle - [\langle \bar{\rho} \tilde{u}_i \rangle \langle \bar{\rho} \tilde{u}_j \rangle] / \hat{\rho} \quad (53)$$

LDKM assumes that the sub-grid stress at the test filter level ( $\hat{\tau}_{ij}^{sgs}$ ) are also similar ( $\hat{\tau}_{ij}^{sgs} = \hat{C}_L L_{ij}$ ). Then  $\hat{\tau}_{ij}^{sgs}$  is modeled using the same form used for  $\tau_{ij}^{sgs}$  with all variables defined at the test filter level. With this assumption the expression for  $L_{ij}$  becomes:

$$L_{ij} = \frac{\hat{\tau}_{ij}^{sgs}}{\hat{C}_L} = 2\hat{\rho} \frac{C_\nu}{\hat{C}_L} \sqrt{k^{test}} \hat{\Delta} \left( \langle \tilde{S}_{ij} \rangle - \frac{1}{3} \langle \tilde{S}_{kk} \rangle \delta_{ij} \right) + \frac{2}{3} \frac{1}{\hat{C}_L} \hat{\rho} k^{test} \delta_{ij} \quad (54)$$

Assuming  $\hat{C}_L = 1$ ,  $C_\nu$  is determined using the least square method of Lilly:

$$C_\nu = -\frac{L'_{ij} M_{ij}}{2M_{ij} M_{ij}} \quad (55)$$

In the above expression,  $L'_{ij} = L_{ij} - \frac{2}{3} \hat{\rho} k^{test} \delta_{ij}$ , and  $M_{ij} = \hat{\rho} \sqrt{k^{test}} \hat{\Delta} \left( \langle \tilde{S}_{ij} \rangle - \frac{1}{3} \langle \tilde{S}_{kk} \rangle \delta_{ij} \right)$ .

A similar approach is used to obtain the dissipation coefficient  $C_\epsilon$ :

$$C_\epsilon = \frac{\hat{\Delta} (\bar{\mu} + \mu_t)}{\hat{\rho} k^{test 3/2}} \left[ \left\langle \tilde{T}_{ij} \frac{\partial \tilde{u}_j}{\partial x_i} \right\rangle - \hat{T}_{ij} \frac{\partial \hat{u}_j}{\partial x_i} \right] \quad (56)$$



where,  $\mu_t = \bar{\rho}\nu_t$ ,  $\tilde{T}_{ij} = \left[ \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3} \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij} \right]$ , and  $\widehat{T}_{ij}$  is the stress tensor at the test filter level. Seven realizability conditions need to be satisfied for a subgrid scale stress tensor to guarantee a realizable solution. These conditions are:

$$(1-3) \tau_{ij} \geq 0, \text{ where } i = 1, 2, 3;$$

$$(4-6) |\tau_{ij}| \leq \sqrt{\tau_{ii}\tau_{jj}}, \text{ where } i \neq j;$$

$$(7) \det(\tau_{ij}) \geq 0.$$

The LDKM approach is ensured to satisfy all the realizability conditions at majority of grid points.

### 2.5.2 Subgrid Combustion Modelling using LEM

In the present study a subgrid combustion model based on LEM is used to account for the combustion occurring within the LES cells (LEMLES, hereafter), since combustion, heat release, volumetric expansion and small-scale turbulent stirring all occur at small scales, which are not resolved in a conventional LES approach. No explicit closure is provided for subgrid mass flux,  $\phi_{i,k}^{sgs}$ , the subgrid diffusive flux,  $\theta_{i,k}^{sgs}$ , and the filtered reaction rate  $\bar{\omega}_k$ , since a more accurate and exact closure is implemented within the subgrid scales.

LEM is a stochastic, Monte-Carlo simulation of the unsteady scalar field evolution in a turbulent flow, based on solving the unsteady reaction-diffusion equation on a one-dimensional domain, treating turbulent convection separately at its own time scale. The computational domain is aligned in the direction of the steepest scalar gradient with grid resolution  $\eta$ . The turbulent field is assumed to be isotropic with no boundaries and/or body forces. In LEM, the molecular diffusion and chemical reaction evolve deterministically from an initial scalar field by the solution of the thermochemical equations.

Consider the following exact transport equation for the  $k$ -th scalar  $Y_k$ , where there is

no spatial filtering:

$$\rho \frac{\partial Y_k}{\partial t} = -\rho \left[ \tilde{u}_i + (u'_i)^R + (u'_i)^S \right] \frac{\partial Y_k}{\partial x_i} - \frac{\partial}{\partial x_i} (\rho Y_k (V_{i,k} + V_i^C)) + \dot{\omega}_k \quad (57)$$

The convective velocity is separated into three parts: the LES resolved velocity field  $\tilde{u}_i$ , the LES resolved subgrid fluctuation (obtained from  $k^{sgs}$ )  $(\tilde{u}_i)^R$ , and the unresolved subgrid fluctuation  $(\tilde{u}_i)^S$ . Using this definition eq. (57) can be split into the following two-step numerical form:

$$\rho \frac{\partial Y_k}{\partial t} = - \left[ (\tilde{u}_i + u'_i)^R \right] \frac{\partial Y_k}{\partial x_i} \quad (58)$$

$$\rho \frac{\partial Y_k}{\partial t} = \rho (u'_i)^S \frac{\partial Y_k}{\partial x_i} + \frac{\partial}{\partial x_i} (\rho Y_k (V_{i,k} - V_i^C)) - \dot{\omega}_k \quad (59)$$

Eqs. (58) and (59) represent large-scale and small-scale processes, respectively. The large-scale step advects the subgrid scalar gradient using a 3D Lagrangian process that ensures strict mass conservation and preserves the small-scale scalar structure. In eq. (59) the three terms represent the small-scale turbulent stirring, molecular diffusion and chemical kinetics, respectively. Eq. (59) is solved on a 1D line embedded inside each LES cells with a subgrid resolution fine enough to resolve the Kolmogorov scale,  $\eta$ , so that both molecular diffusion and reaction rate are closed in an exact sense.

Based on this approach, in the LEMLES model the following reaction-diffusion equation is solved on the 1D LEM level:

$$\begin{aligned} \rho \frac{\partial Y_k}{\partial t} &= F_{k, stir} - \frac{\partial}{\partial s} (\rho Y_k (V_{k,s} - V_k^C)) + \dot{\omega}_k \\ \rho C_p \frac{\partial T}{\partial t} &= F_{T, stir} - \rho \frac{\partial T}{\partial s} \left( \sum_{k=1}^{N_s} C_{p,k} Y_k (V_{k,s} - V_s^C) \right) + \frac{\partial}{\partial s} \left( \kappa \frac{\partial T}{\partial s} \right) + \dot{\omega}_T \end{aligned} \quad (60)$$

In this equation, heat release due to combustion is calculated as  $\dot{\omega}_T = - \sum_{k=1}^{N_s} h_k \dot{\omega}_k W_k$ . The subgrid field within each LES supergrid is resolved by  $N_{LEM}$  number of cells along the local coordinate  $s$ , aligned in the direction of the steepest gradient.

### 2.5.2.1 Small Scales: Turbulent Stirring

Within LEM, turbulent stirring is solved stochastically by a numerical re-arrangement event known as triplet-maps, represented symbolically by  $F_{k, stir}$  and  $F_{T, stir}$  in Eq. (60). It is based on the assumption that the effect of the turbulent eddies on the scalar field is to stochastically redistribute the concentration gradients, by only increasing the scalar gradients. Hence, for a given initial scalar profile, the turbulent advection increases the gradients by re-distribution process whereas molecular diffusion competes with it by smoothing out these gradients. Schematically, this mapping first creates three copies of the selected segment by a factor of three and reversing the middle segment.

The location of stirring event is chosen randomly from a uniform distribution and the frequency of stirring is implemented as a Poisson process in time [19] as:

$$\lambda = \frac{54 \nu Re_{\bar{\Delta}}}{5 C_{\lambda} \bar{\Delta}^3} \frac{\left[ \left( \frac{\bar{\Delta}}{\eta} \right)^{5/3} - 1 \right]}{\left[ 1 - \left( \frac{\eta}{\bar{\Delta}} \right)^{4/3} \right]} \quad (61)$$

where,  $C_{\lambda} = 0.067$  [5]. The eddy size ( $l$ ) is picked randomly from an eddy distribution  $f(l)$  ranging from  $\bar{\Delta}$  to  $\eta$ :

$$f(l) = \frac{5}{3} \frac{l^{-8/3}}{(\eta^{-5/3} - \bar{\Delta}^{-5/3})} \quad (62)$$

where  $\eta = N_{\eta} \bar{\Delta} Re_{\bar{\Delta}}^{-3/4}$  and  $Re_{\bar{\Delta}} = u' \bar{\Delta} / \nu$  is the subgrid Reynolds number.

### 2.5.2.2 Volumetric expansion

The volumetric expansion in LEM is implemented locally within the subgrid by expanding the LEM domain and after splicing re-gridding is done to keep the total number of LEM constant within each cell.

### 2.5.2.3 Large Scales: Advection

After the evolution of the subgrid scalar field, large scale advection is implemented by a 3D Lagrangian process known as splicing that determines the amount of mass

to be advected and advects this amount with the subgrid scalar fields across the LES cell faces.

### 2.5.3 Subgrid Combustion Modelling directly within LES

In the LES simulation  $\theta_{i,k}^{sgs}$  is neglected and the  $\phi_{i,k}^{sgs}$  is modelled  $\phi_{i,k}^{sgs} = -\frac{\bar{\rho}\nu_t}{Sc_t} \frac{\partial \tilde{Y}_k}{\partial x_i}$ . For the filtered reaction rate  $\bar{\omega}_k$  some form of closure is required. This closure is discussed in details later.

## CHAPTER III

### PROBLEM SETUP

Two cases corresponding to a low and a high  $Re$ , are chosen as test cases from the previous DNS study [14] of 3D turbulent temporally evolving syngas(CO/H<sub>2</sub>)-air diffusion flames. These cases exhibit local extinction and reignition as a result of strong flame-turbulence interaction and poses a challenging problem for the TANN methodology. Both the LES and DNS study employ the same setup.

#### *3.1 Problem Description*

The central fuel stream, of width  $H$ , is composed of 50% CO, 10% H<sub>2</sub> and 40% N<sub>2</sub> by volume. Surrounding the central fuel stream are counter-flowing oxidizer streams composed of 25% O<sub>2</sub> and 75% N<sub>2</sub>. The domain size is  $L_X = 12H$  in stream-wise direction,  $L_Y = 14H$  in the transverse direction and  $L_Z = 8H$  in the span-wise direction. The boundary conditions are periodic, non-reflecting outflow and periodic in the stream-wise, transverse and span-wise directions, respectively. The details of the two DNS cases are give in table 1.

The LES study employs grids clustered near the shear layer in the flame normal direction with smooth stretching towards the transverse boundaries, while uniform spacing is used in the other two directions because the gradients are highest across

**Table 1:** DNS parameters for test cases

Parameter	Case L	Case H
$H(mm)$	0.72	1.37
$Re_{jet}$	2510	9079
Grid Size (M)	148	500
Grid Resolution	$0.83\eta$	$1.67\eta$

**Table 2:** LES parameters for test cases

Grid Resolution	Size	min. $\Delta y$	max. $\Delta y$
Case L	$90 \times 126 \times 50$ ( $0.56M$ )	0.055 mm	0.152 mm
Case H (C-GRID)	$120 \times 180 \times 90$ ( $1.9M$ )	0.045 mm	0.218 mm
Case H (M-GRID)	$160 \times 240 \times 120$ ( $4.6M$ )	0.035 mm	0.161 mm
Case H (F-GRID)	$200 \times 300 \times 150$ ( $9M$ )	0.028 mm	0.129 mm

the flame in the flame normal direction. The details of the LES setup is given in table 2. Like the DNS study, the LES is initialized with a laminar flamelet solution at a scalar dissipation rate  $\chi = 0.75\chi_q$  ( $\chi_q = 2194s^{-1}$ , extinction scalar dissipation rate). For calculating the heat and species diffusion fluxes mixture-averaged transport properties are used.

## CHAPTER IV

### RESULTS

#### *4.1 ANN Net Generation*

One LANN net and three TANN nets: TANN-1, TANN-2 and TANN-3 are generated. Training data for LANN and TANN-1 is generated from a 1D stand-alone LEM simulation (Stand-alone LEM 1). Training data for TANN-2 and TANN-3 is generated from another stand-alone simulation run over a larger range of  $Re_t$  (Stand-alone LEM 2). Both the standalone LEM simulations are initialized with the same OPPDIFF flame obtained from Chemkin.

Stand-alone LEM 1 is simulated for  $Re_t$  up to 1000. Instantaneous thermochemical data is tabulated at regular intervals for generating the training table for LANN. For generating the training table for TANN-1, the data on the 1D stand-alone LEM domain is filtered over a fixed filter size of 0.1 mm and time step size of  $2.5 \times 10^{-8}s$ . The filter size and time step size is representative of the Case L LES grid size and time step size. In order to generate TANN capable of handling a larger range of  $\chi$ , stand-alone LEM 2 is simulated for  $Re_t$  up to 1500. A fixed filter size of 0.042 mm and time step size of  $1.0 \times 10^{-8}s$  are chosen to generate the training table for TANN-2. The filter size is representative of the average grid size for all the four LES cases and the time step size is smaller than the time step size for finest LES grid. This time step size is enforced for all LES simulations while using TANN-2 and TANN-3. For generating the training table for TANN-3, the training table for TANN-2 is re-tabulated with the species dissipation rate instead of species gradient.

For training the ANN nets, the training data is split into two tables Train and Test. The Train table gets 80% of the data and Test table gets 20%. The data in the Train

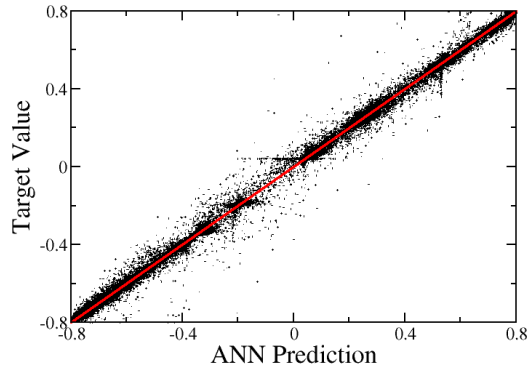
table is used for training the net. Once the training is complete, data in the Test table is used for comparing the source term obtained from ANN with the source term tabulated from the stand-alone LEM simulation. This gives an estimate about how the ANN net will perform at thermochemical data points for which it has not been trained.

Choosing the ANN architecture with the correct number of hidden layers and number of processing elements in each hidden layer is a challenging task. Two or more number of hidden layers is required for modelling complex data with discontinuities. If an inadequate number of processing elements are used in a hidden layer, the net will not be able to model complex data. On the other hand, if too many neurons are used, training time will become excessively long and the model may memorize the data. This result in ANN net fitting the data for which it is trained extremely well but generalizing poorly to new unseen data. In the present study all the 4 nets are trained with 3 hidden layers. The LANN is trained with 5, 4 and 3 processing elements in 1st, 2nd and 3rd hidden layers. The LANN has 12 processing elements in the input layer, 1 for the each of the 11 species ( $H_2, O_2, OH, O, H_2O, H, HO_2, CO, CO_2, HCO, N_2$ ) and the 12th for temperature. Since, pressure is a constant in the present study; it is not used as an input. The TANN nets are trained with 10, 8 and 4 processing elements in the 1st, 2nd and 3rd hidden layers. The TANN input layer has 14 processing elements in the input layer, 11 for the species, 12th for the temperature, 13th for turbulent Re and the last one for species gradient in case of TANN-1 and TANN-2, and species dissipation rate for TANN-3. These architectures are chosen based on a previous study[32]. To prevent memorization of data by the ANN, it is necessary to stop the training at the correct time, once the training error does not change significantly with further iterations. In the present study, the training is stopped if the training error does not decrease after a given number of iterations.



## 4.2 Verification of the accuracy of the nets

After the training of the ANN net is complete and the weight distribution is optimum, to verify the accuracy of the network, the target values for the source term from the Test table are compared with the values predicted by the ANN network. Fig. 4 shows the comparison of the Target values and ANN predicted values for TANN-2 net. All the data points would have fallen on red line had the training been perfect. It is observed that there is some deviation from the red line. Most points show very little deviation from the red line and very few points show large deviation from the red line. Overall, TANN-2 predicts ANN values very close to target values for most of the test data points and the training is good. Similar trends are observed for the Target vs. ANN predicted values for other nets. Hence, all the four ANN nets are trained well.



**Figure 4:** Comparison of Target vs. ANN prediction using TANN-2

## 4.3 Difference between LANN and TANN

The LANN is capable of calculating the instantaneous source terms within the LEM subgrid combustion model in LES framework as:

$$\frac{\dot{\omega}_i}{\rho} = f(Y_1, \dots, Y_{N_s}, T) \text{ where, } i=1, \dots, N_s \quad (63)$$

for a fixed  $\Delta t$  and pressure.

TANN-1 and TANN-2 can compute the filtered source terms directly within the LES framework as:

$$\frac{\bar{\dot{\omega}}_i}{\bar{\rho}} = f \left( \tilde{Y}_1, \dots, \tilde{Y}_{N_s}, \tilde{T}, Re_\Delta, \frac{\partial \tilde{Y}_i}{\partial x_j} \right) \text{ where, } i=1, \dots, N_s \quad (64)$$

for a fixed  $\Delta t$ , pressure and filter size representative of LES grid size.

TANN-3 can compute the filtered source terms directly within the LES framework as:

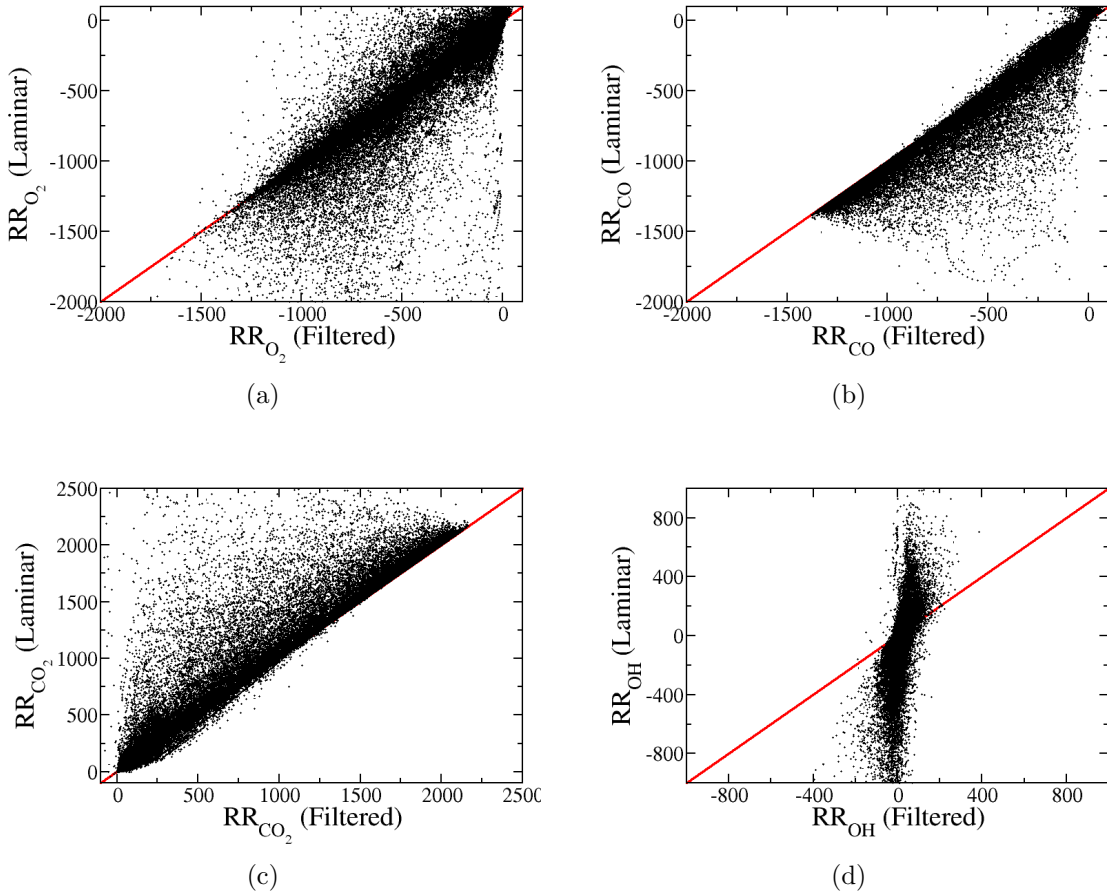
$$\frac{\bar{\dot{\omega}}_i}{\bar{\rho}} = f \left( \tilde{Y}_1, \dots, \tilde{Y}_{N_s}, \tilde{T}, Re_\Delta, 2D_i \frac{\partial \tilde{Y}_i}{\partial x_j} \cdot \frac{\partial \tilde{Y}_i}{\partial x_j} \right) \text{ where, } i=1, \dots, N_s \quad (65)$$

for a fixed  $\Delta t$ , pressure and filter size representative of LES grid size.

The TANNs are trained as a function of the subgrid Re and filtered species gradient or filtered species dissipation rate, in addition to the filtered species mass fractions and filtered temperature. This is done to take into account the effect of turbulence and subgrid mixing. To evaluate if there is any difference between the laminar (instantaneous) reaction rates and the filtered (turbulent) reaction rates, filtered reaction rates obtained from the stand-alone LEM are compared with the instantaneous reaction rates for the same composition and time step size, as shown in Fig. 5. To obtain the filtered reaction rates, the filtered mass fractions are calculated at a given instant of time and at an instant after the LES time step size, on the standalone LEM domain. Their difference divided by the LES time step size gives the filtered reaction rate. To compute the instantaneous reaction rate, the instantaneous mass fractions and temperature are taken as input. Then direct integration is used to compute the instantaneous reaction rates. It is observed that the production of CO<sub>2</sub> and the consumption of O<sub>2</sub> and CO is faster for laminar chemistry compared to the turbulent chemistry. For OH radical, the magnitude of the laminar reaction rates is much higher, compared to the filtered reaction rate. The other radicals also show

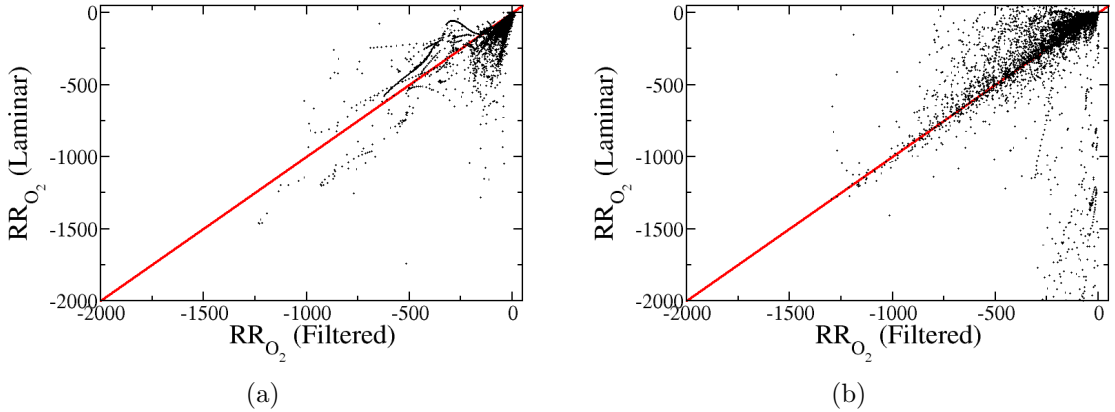
similar trend like OH. OH laminar reaction rates vary from -800 to +800, approximately and OH filtered reaction rates varies from -200 to +200, approximately. This indicates that OH radicals are produced and consumed at almost the same rate in a given chemistry. This keeps their concentration low. However, their rate of production and consumption with laminar chemistry is higher than turbulent chemistry. Overall, the laminar chemistry assumption predicts faster combustion compared to the turbulent chemistry because the laminar chemistry does not take into account the effect of turbulence and the high scalar dissipation rates, which leads to fast removal of heat and the radicals from the reaction zone and thus drop in the heat release rate.

Fig. 6(a) and 6(b) show the comparison between filtered reaction rate and the



**Figure 5:** Comparison of the filtered reaction rates and the laminar reaction rates for (a)  $O_2$ , (b)  $CO$ , (c)  $CO_2$ , (d)  $OH$ .

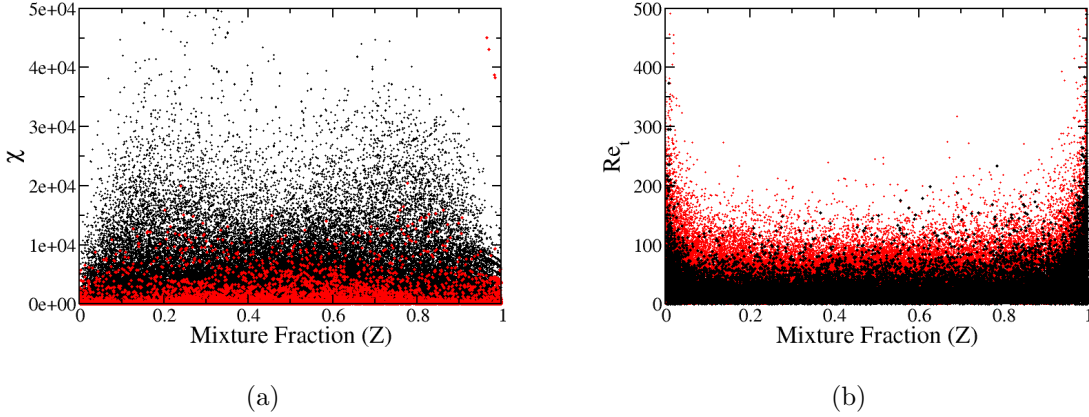
laminar reaction rate of  $O_2$  for low and high scalar dissipation rates. More difference between the laminar reaction rate and the filtered reaction rate is observed for higher scalar dissipation rates due to stronger turbulence-chemistry interactions which leads to chemical time scales comparable with the diffusion time scales and thus laminar chemistry assumption is no longer valid. Hence, the source term predicted by LANN used directly within the LES framework is different from the source term predicted by TANN used within the LES framework.



**Figure 6:** Comparison of the filtered reaction rates and the laminar reaction rates for  $O_2$  at (a)  $\chi < 1.0s^{-1}$ , (b)  $\chi > 1000s^{-1}$ .

#### 4.4 Comparison of TANN-1 and TANN-2 training data

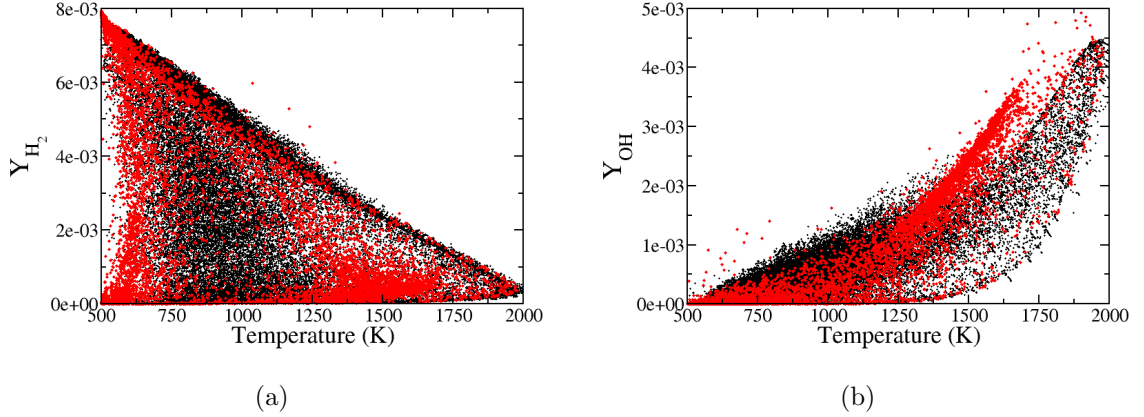
Fig. 7(a) shows the comparison of  $\chi$  with respect to  $Z$  for the standalone LEM data tables used for training the two nets TANN-1 and TANN-2. The standalone LEM data used for training TANN-1 was generated using a lower  $Re_t$  and larger filtered grid spacing compared to TANN-2 as explained in the previous section. As a result of higher  $Re_t$  and smaller grid spacing used for training TANN-2 compared to TANN-1, the  $\chi$  values for TANN-2 are much higher. The TANN-1 and TANN-2 training data explore a maximum  $\chi$  close to 20,000 and 50,000, respectively. Fig. 7(b) shows the



**Figure 7:** Comparison of the standalone LEM data used for training the nets. Red symbols: TANN-1, Black symbols: TANN-2. (a)  $\chi$  vs  $Z$ , (b)  $Re_t$  vs  $Z$

comparison of  $Re_t$  with respect to  $Z$  for the two training data tables. It is observed that the  $Re_t$  values explored by TANN-1 are slightly higher than the  $Re_t$  values explored by TANN-2 because  $Re_t$  is directly proportional to the grid spacing and the grid spacing for TANN-2 is lower than the grid spacing for TANN-1.

Fig. 8(a) and 8(b) show the comparison of mass fraction of  $H_2$  and  $OH$  with respect to temperature for the two training tables. The thermochemical data space covered by mass fraction of  $H_2$ , for the two training tables are very similar and overlap with each other. However, the thermochemical data space of  $OH$  does not overlap very well beyond a mass fraction of  $2.5 \times 10^{-3}$ . It is shown in the discussions later that the maximum  $OH$  mass fraction covered by the two LES test cases is around  $2.5 \times 10^{-3}$ . Hence, the region of mismatch for the  $OH$  thermochemical data space lies outside the area of interest for the two test cases. Therefore, based on the comparison of the training data for the two nets it is observed that even though the compositional data space explored by the two training tables are the same, the  $\chi$  and  $Re_t$  data space differ. Hence, TANN-2 covers a wider range of  $\chi$  compared to TANN-1 and is a more "generalized" net.



**Figure 8:** Comparison of the standalone LEM data used for training the nets. Red symbols: TANN-1, Black symbols: TANN-2. (a)  $H_2$  mass fraction vs  $Z$ , (b)  $OH$  mass fraction vs  $Z$

#### 4.5 Comparison of TANN-2 and TANN-3

TANN-2 and TANN-3 nets are trained on the same stand-alone LEM data. The only difference between the nets is TANN-2 computes the filtered source term as a function of species gradient whereas TANN-3 computes the source term as a function of species dissipation rate. The species dissipation rate is a function of the molecular diffusivity  $D$  in addition to species gradient and it plays an important role when the species in the reaction zone have a large range of molecular diffusivity. The lighter species like  $H$ ,  $H_2$  have higher molecular diffusivity than heavier species like  $CO$ ,  $CO_2$ . Hence, for the same species gradient lighter species have a higher species dissipation rate compared to heavier species. Thus, TANN-3 takes into account the effect of variable species diffusivity in addition to the species gradient.

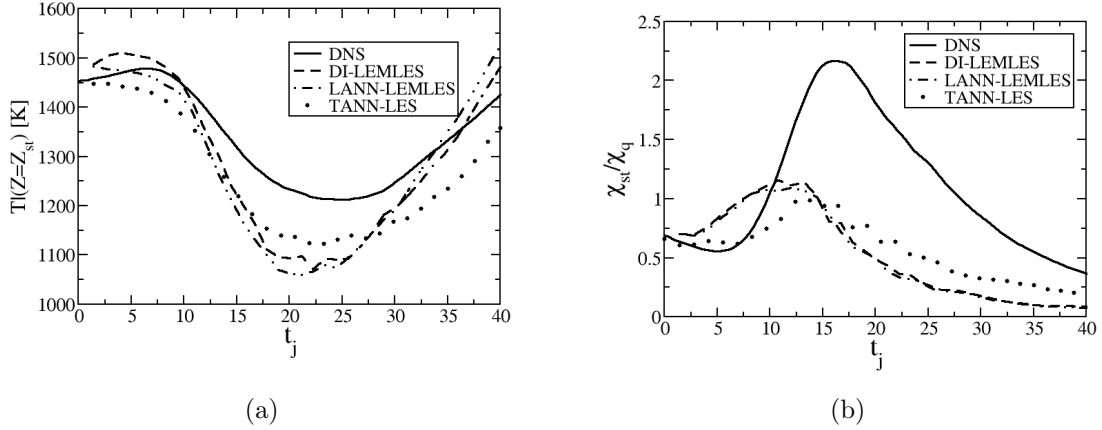
#### 4.6 Case L: TANN-LES validation

To assess the performance of TANN methodology, the Case L is run with DI-LEMLES, LANN-LEMLES and TANN-LES using the TANN-1. Fig. 9(a) shows the variation of the mean temperature on the stoichiometric plane with respect to the non-dimensional-time ( $t_j$ ) for DNS, DI-LEMLES, LANN-LEMLES and TANN-LES. The time is non-dimensional by the reference time obtained as  $t^* = H/U$ , where  $U$  is the already defined characteristic jet velocity [14]. The DNS data shows that the temperature begins at 1455 K and drops off to a minimum of approximately 1210 K near  $t_j = 20$ , indicating extinction. Beyond this point the temperature starts increasing again and reaches 1425 K at  $t_j = 40$ , showing complete reignition. The DI-LEMLES initially over predicts the temperature till  $t_j = 10$  beyond which it drops off faster than the DNS temperature profile. LANN-LEMLES and TANN-LES almost at all instants till  $t_j = 20$  under predict the mean temperature. The DI-LEMLES, LANN-LEMLES under predict the temperature by approximately 12% and the TANN-LES under predicts the temperature by approximately 8% at  $t_j = 20$ , indicating more extinction compared to DNS. Beyond this point, the temperature on the stoichiometric plane for DI-LEMLES and LANN-LEMLES increases at a higher rate compared to DNS temperature profile, while the TANN-LES stoichiometric plane temperature always remains lower than the DNS. At  $t_j = 40$  the DI-LEMLES, LANN-LEMLES over predict the temperature by approximately 6% and TANN-LES under predicts the temperature by approximately 4%. The LES results highly under predict the temperature on the stoichiometric plane compared to DNS. In DNS, isotropic turbulence is added in the shear layer along a thickness lesser than the minimum LES grid size. Hence, when isotropic turbulence is added in the shear layer in LES it is done along a larger thickness.

Fig. 9(b) shows the variation of the mean  $\chi_{st}/\chi_q$  on the stoichiometric plane with respect to  $t_j$ . The DNS simulations initializes at  $\chi_{st}/\chi_q = 0.75$  (approx.) and increases

to 2.16 at  $t_j = 16$  due to the shear generated turbulence. Beyond this point it starts decaying and drops off to 0.35 at  $t_j = 40$ .

Comparing Fig. 9(a) and 9(b) it is observed that the local extinction is due to the



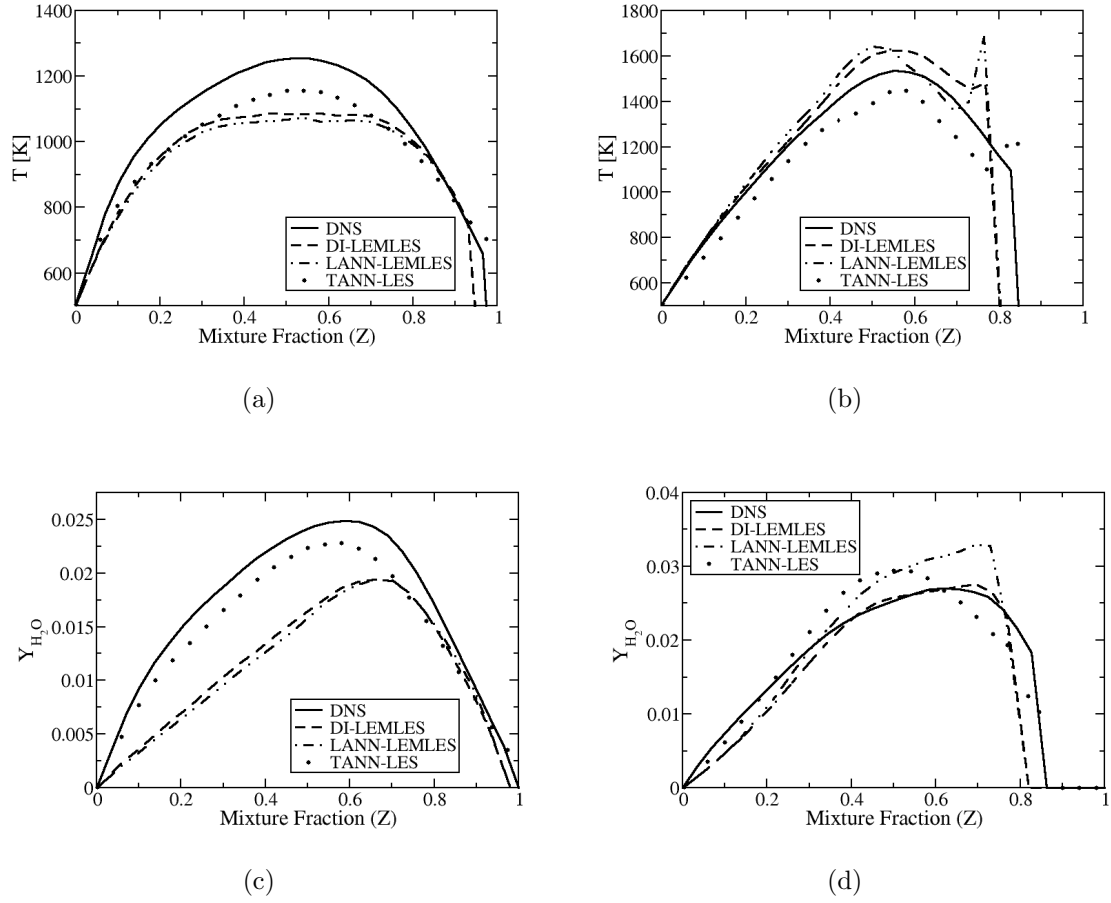
**Figure 9:** (a) Variation of the mean of temperature at stoichiometric mixture fraction with respect to non-dimensional time for Case L, (b) Variation of the mean  $\chi/\chi_q$  at stoichiometric mixture fraction with respect to non-dimensional time for Case L

fluctuations of the scalar dissipation rate. Once the molecular mixing overcomes the effect of turbulent straining, it leads to the decrease of the scalar gradients which is accompanied by gradual reignition [37]. A time lag is observed between the maximum  $\chi_{st}/\chi_q$  and the minimum temperature on the stoichiometric plane because the reaction rate does not immediately follow variations of  $\chi_{st}$  due to the finite rate chemistry [38],[26]. The temperature, at extinction is under predicted by 150K compared to DNS even though  $\chi_{st}$  for LES is lower than the DNS by 100%. The reason the scalar dissipation is so much lower is LES is because it is using a much coarser grid and as Fig. 3 shows the gradient of  $Z$  appear lower on the filtered grid because it is not showing the subgrid fluctuations. So a coarser grid will always show a scalar dissipation rate lower than a fine-grid even though it takes into account the subgrid fluctuations in LEM or by computing the source term as a function of the gradient of the species at filtered level. The DI-LEMLES and LANN-LEMLES predict a faster



initial rate of growth of mean  $\chi_{st}/\chi_q$  compared to the DNS, while the TANN-LES predicts a slower initial rate of growth of  $\chi_{st}/\chi_q$ . The maximum mean  $\chi_{st}/\chi_q$  observed is approximately 1.1 and close to  $t_j = 12$  for DI-LEMLES and LANN-LEMLES, while the maximum mean  $\chi_{st}/\chi_q$  for TANN-LES is observed close to  $t_j = 15$  and has a value of 1 approximately. Beyond this point  $\chi_{st}/\chi_q$  decays off and reaches a value less than 0.2 at  $t_j = 40$  for DI-LEMLES and LANN-LEMLES, while it has a value of 0.25 approximately for TANN-LES. The TANN-LES under predicts  $\chi_{st}/\chi_q$  compared to LEMLES till  $t_j = 15$  and after that it slightly over predicts. Overall the data obtained from TANN-LES is in good agreement with DI-LEMLES data. A similar assessment of case M having  $Re = 4478$  [14] was done in an earlier study [32] and not shown here.

The mean value of temperature and H<sub>2</sub>O mass fraction conditioned on the mixture fraction at extinction ( $t_j = 20$ ) and reignition ( $t_j = 40$ ) are shown in Fig. 10, with DNS, DI-LEMLES, LANN-LEMLES and TANN-LES using TANN-1. At extinction  $t_j = 20$ , the LES results under predict the mean temperature at almost all values of  $Z$  compared to the DNS. Above  $Z = 0.95$  TANN-LES slightly over predicts the mean temperature. Overall, the TANN-LES mean temperature profile shows good match with the DNS temperature profile. Both LES and DNS show that the maximum value of  $Z$  observed for DI-LEMLES and LANN-LEMLES is 0.93. For TANN-LES the maximum value of  $Z$  observed is 0.975 and for DNS it is 0.97. Thus, DI-LEMLES and LANN-LEMLES overpredict mixing while TANN-LES slightly under predict it because of neglecting the subgrid diffusion term, compared to DNS, at extinction. A similar trend in mixture fraction is observed at reignition  $t_j = 40$  and the maximum value of  $Z$  for DNS drops to 0.83. DI-LEMLES and LANN-LEMLES over predicts the mean temperature profile whereas TANN-LES under predicts the temperature profile at almost all values of  $Z$ , at reignition. The maximum temperature at both  $t_j = 20$  and  $t_j = 40$  is observed on the fuel-rich side instead of stoichiometric plane.

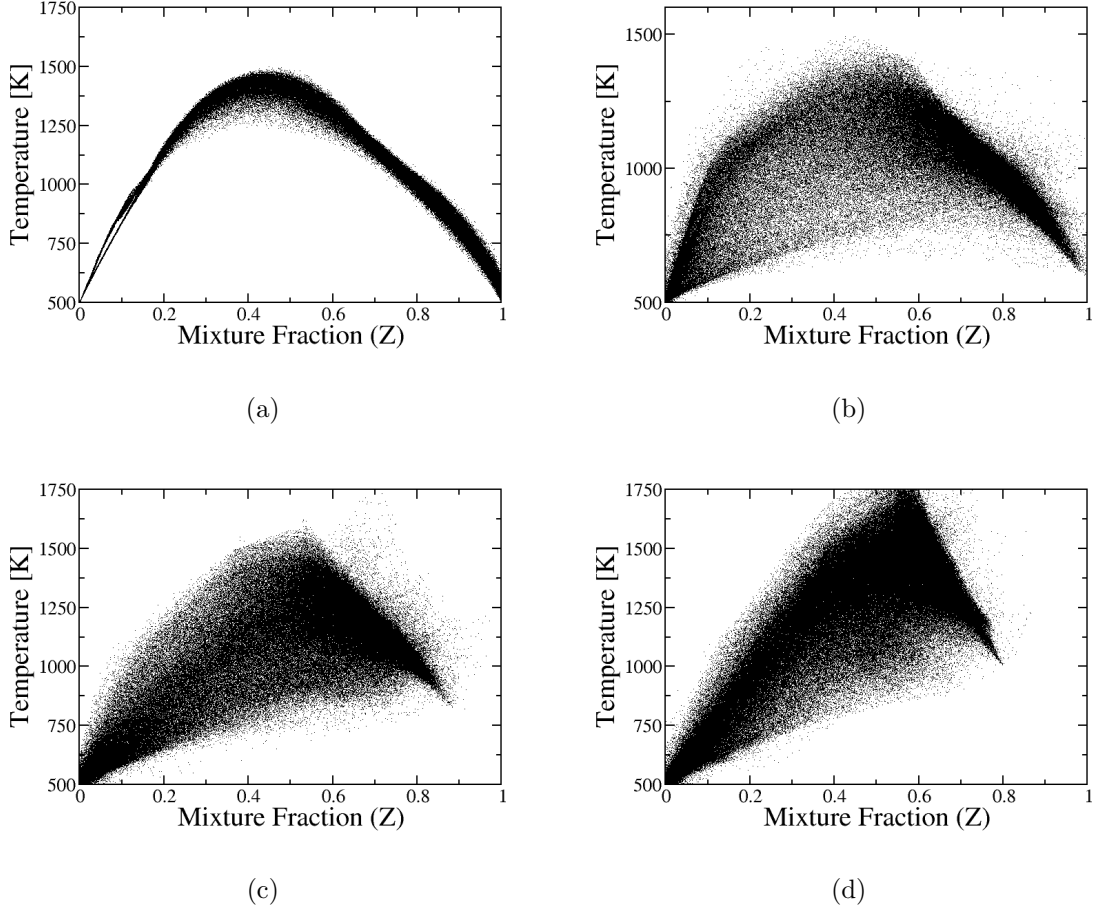


**Figure 10:** Conditional mean of temperature and  $Y_{H_2O}$  at extinction (a and c) and reignition (b and d)

This is observed due to the significant differential diffusion effect which leads to higher diffusion velocities of lighter species like H, H<sub>2</sub>, OH and O compared to other species. The radicals diffuse more towards the fuel side and shift the location of the maximum heat release also making the heat release zone wider [15]. At extinction, the H<sub>2</sub>O mass fraction is under predicted for all values of Z by the LES simulations. DI-LEMLES and LANN-LEMLES under predicts the production of H<sub>2</sub>O more whereas TANN-LES under predicts it less compared to the DNS, which is consistent with the temperature profile predictions suggesting more extinction compared to the DNS and thus lower heat release rate and less production of products. The location of the maximum mass fraction of H<sub>2</sub>O lies in the fuel-rich side, around 0.6 for DNS and TANN-LES and

around 0.7 for DI-LEMLES and LANN-LEMLES due to differential diffusion effects. The DNS data shows that maximum mass fraction of  $\text{H}_2\text{O}$  increases from 0.025 to 0.027 at  $t_j = 20$  to  $t_j = 40$ . The LES results over predict the maximum mass fraction of  $\text{H}_2\text{O}$  at reignition compared to DNS.

Fig. 11 shows the time evolution of the scatter cloud of temperature with respect

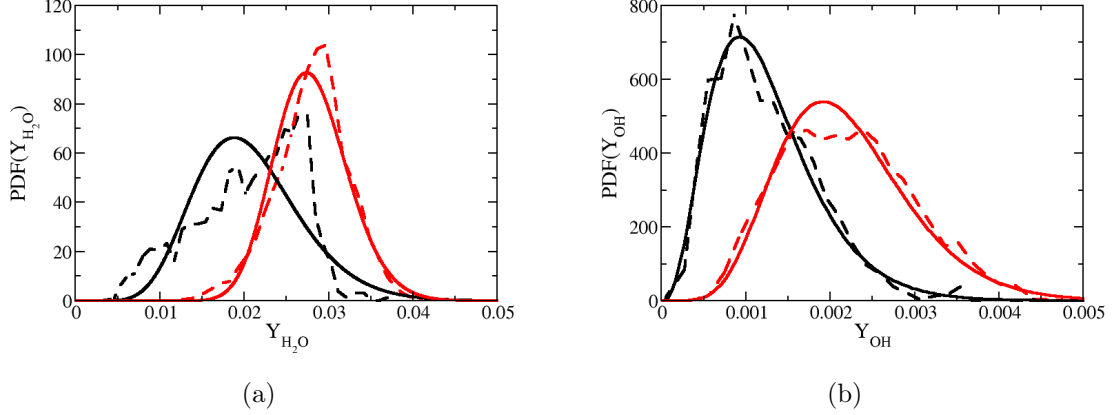


**Figure 11:** Case L, TANN-LES using TANN-1: Evolution of temperature w.r.t.  $Z$  at  $t_j$  a)10, b)20, c)30 and d)40.

to mixture fraction. At  $t_j = 10$  a small scatter about the mean is observed. By  $t_j = 20$  the scatter increases along with a drop in the mean temperature. At  $t_j = 30$  and  $t_j = 40$  the scatter reduces along with an upward shift of the cloud. The initial increase in the scatter and drop in the mean stoichiometric plane temperature at  $t_j = 20$  followed by decrease in scatter and upward shift of the cloud at  $t_j = 40$

indicates the extinction-reignition phenomenon.

Fig. 12(a) and 12(b) show the pdf of the  $H_2O$  and  $OH$  mass fraction at extinction



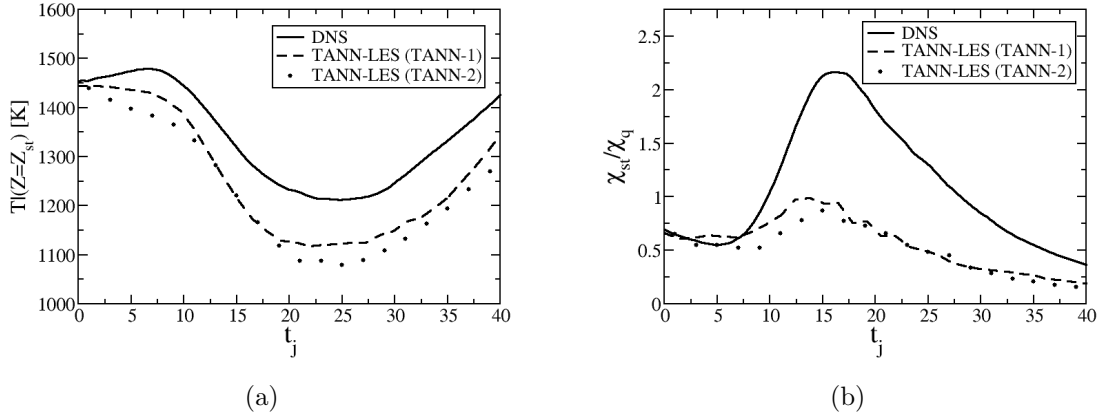
**Figure 12:** Case L, TANN-LES using TANN-1: pdf on stoichiometric plane at extinction and reignition of a)  $H_2O$ , b)  $OH$ . Black continuous line: extinction ( $t_j = 20$ ), black broken line:  $\beta$ -pdf at extinction, red continuous line: reignition ( $t_j = 40$ ), red broken line:  $\beta$ -pdf at reignition,

( $t_j = 20$ ) and reignition ( $t_j = 40$ ) for TANN-LES using TANN-1. The pdf of  $H_2O$  shows more deviation from the beta-pdf at extinction than at reignition. This is in agreement with the observations made by Goldin et al. [13],[12] Near extinction due to the large values of  $\chi$  on the stoichiometric plane the rate of diffusion of species is comparable with the chemical reaction rates resulting in high levels of chemical non-equilibrium which leads to scalar field deviation from the beta-pdf. At  $t_j = 40$ , once the mean  $\chi_{st}$  has dropped off the system once again approaches chemical equilibrium and the pdf shows good agreement with the beta-pdf. The  $OH$  pdf matches well with the beta-pdf at both extinction and reignition because the chemical time scales of  $OH$  radical is small and hence  $OH$  mass fraction stays close to equilibrium at both extinction and reignition.

From the above studies it is concluded that the TANN-LES is a robust methodology and the results predicted by it compare well with the DNS, DI-LEMLES and LANN-LEMLES predictions. For all the results reported hereafter only TANN-LES

computations were done.

To show that TANN-2 (which is more "generalized" compared to TANN-1) is capable of handling a range of  $Re$ , case L is simulated with TANN-LES using TANN-2. Fig. 13(a) and 13(b) show the comparison of the temporal variation of mean temperature and mean  $\chi_{st}/\chi_q$  on the stoichiometric plane for case L using TANN-1 and TANN-2. Both TANN-1 and TANN-2 under predict the temperature on the stoichio-



**Figure 13:** Comparison of the variation of (a) mean temperature and (b) mean  $\chi/\chi_q$  on the stoichiometric plane for Case L using TANN-1 and TANN-2

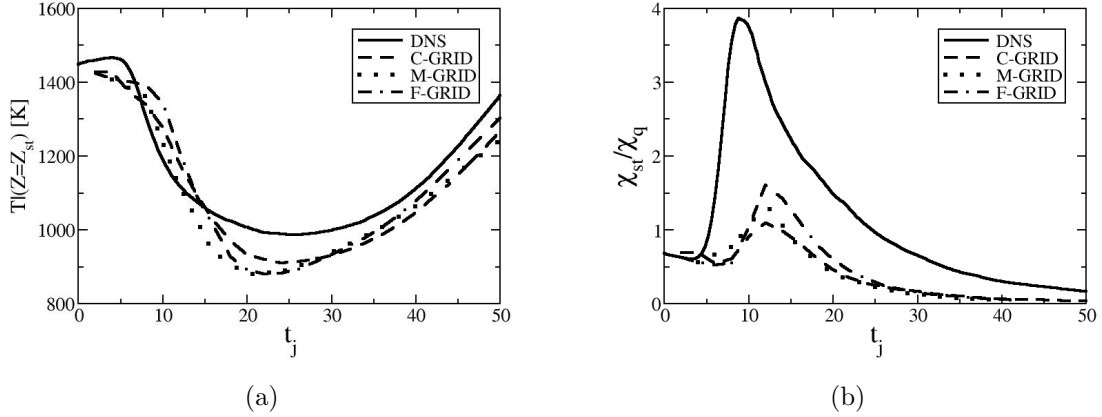
metric plane throughout the course of the simulation. TANN-1, trained on a smaller range of  $Re_t$  and grid-size matching with case L predicts a solution closer to DNS compared to TANN-2, trained on a wider range of  $Re_t$  and smaller grid spacing. The mean  $\chi_{st}/\chi_q$  is slightly under predicted by TANN-2 compared to TANN-1 till  $t_j = 15$ , beyond which the TANN-1 results almost overlap with TANN-2 results. Overall the TANN-1 and TANN-2 results match well for case L and loss of accuracy by using the generalized net TANN-2 compared to the case specific net TANN-1 is negligible.

#### 4.7 Case H: Grid independence study using a single TANN net

The TANN-1 failed to predict extinction-reignition for Case H. TANN-2 generated for a larger range of  $Re_t$  as mentioned earlier successfully simulated Case H.

Fig. 14(a) and 14(b) show the variation of the mean temperature and mean  $\chi_{st}/\chi_q$  on the stoichiometric plane with respect to  $t_j$  for DNS and TANN-LES using TANN-2 for Case H C-GRID, M-GRID and F-GRID. Variation in the grid refinement results in F-GRID estimating the highest mean  $\chi_{st}/\chi_q$  and the C-GRID the lowest because a finer grid captures the subgrid fluctuations better. All the grids for case H predict the highest mean  $\chi_{st}/\chi_q$  around  $t_j = 12$  which is slightly later in time compared to the prediction of DNS. After  $t_j = 15$  the temperature field is slightly under predicted by all the three grids compared to the DNS data. Like DNS the extinction and reignition are observed at  $t_j = 25$  and  $t_j = 50$ , respectively, even though the temperature at extinction is slightly under predicted. The lower mean temperature at extinction and longer reignition time, in case H compared to case L, is observed due to the higher levels of initial turbulence [14]. Overall, the mean temperature predictions for the three grids are reasonably consistent and compare well with the DNS data. Unlike Case L, the temperature on stoichiometric plane compare well for Case H C-GRID. Because the LES cell thickness size in shear layer for Case H C-GRID is smaller than Case L and in Case H, isotropic turbulence is added over a larger thickness. Hence, there is lesser mismatch in isotropic turbulence addition between DNS and LES in Case H compared to Case L.

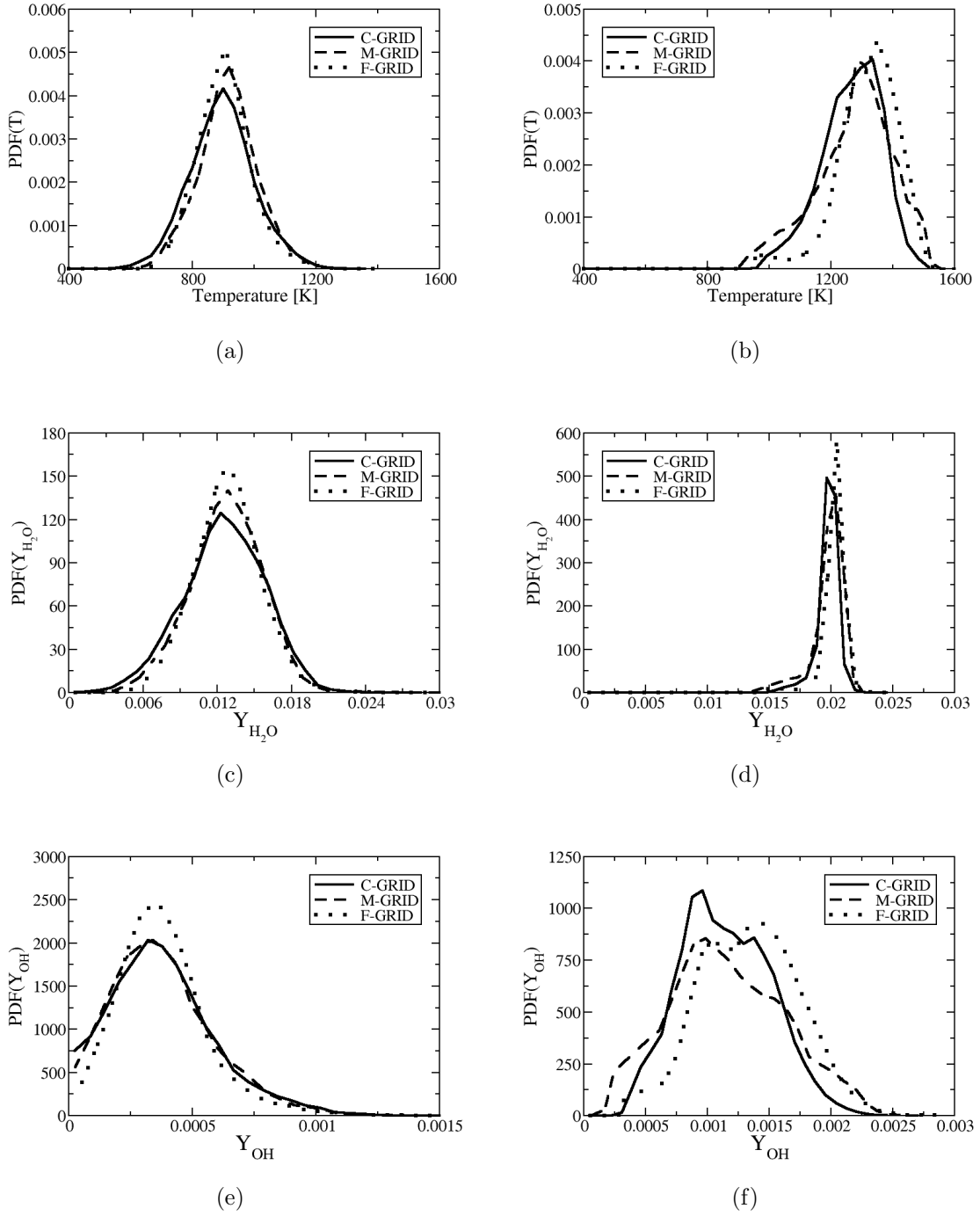
Fig. 15 show the comparison of the pdfs of temperature,  $H_2O$  and  $OH$  mass fractions at extinction( $t_j = 25$ ) and reignition( $t_j = 50$ ) on the stoichiometric plane for C-GRID, M-GRID, F-GRID. The pdf profile of temperature at  $t_j = 25$  for all the three grids compare well with each other having the mean around 900K with slight narrowing of the pdf from C-GRID to F-GRID. At  $t_j = 50$  the mean of all the three pdfs shift



**Figure 14:** Case H (a) Variation of the mean of temperature at stoichiometric mixture fraction with respect to non-dimensional time, (b) Variation of the mean  $\chi/\chi_q$  at stoichiometric mixture fraction with respect to non-dimensional time

to 1300K with the low temperature tail subsiding. The F-GRID exhibits a more prominent low temperature tail suggesting the presence of more reignition compared to the other two cases. At  $t_j = 25$ , the pdf of the mass fraction of both  $H_2O$  and OH compare well with each other and the mean lie around 0.012 and 0.0004 for  $H_2O$  and OH respectively. At  $t_j = 50$  the  $H_2O$  pdf narrows down and the mean  $H_2O$  and OH increases to 0.02 and 0.0012, respectively. Hence, these pdfs clearly exhibit the extinction-reignition process.

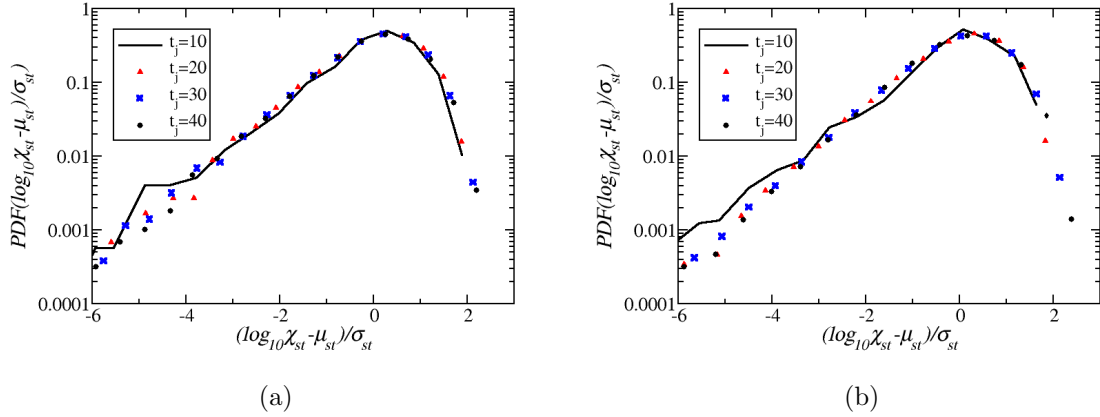
Fig. 16(a) and 16(b) show the comparison of the pdf of the normalized  $\chi_{st}$  at different instants of time for C-GRID and F-GRID, respectively. Maximum negative skewness is observed at  $t_j = 10$  where the mean  $\chi_{st}$  is maximum for both the cases. The negative skewness is observed because at high values of mean  $\chi_{st}$  only at very limited number of points on the stoichiometric plane the  $\chi$  reaches very high values and shift the mean. At majority of the points on the stoichiometric plane the  $\chi$  values lie below the mean and hence result in negative skewness. This phenomenon is explained in Fig. 17(a) and 17(b), which show the distribution of  $\chi$  with respect to temperature on the stoichiometric plane for C-GRID and F-GRID, respectively. At  $t_j = 10$  maximum points lie below mean  $\chi_{st}$  value of 2000 and 2300 for C-GRID and



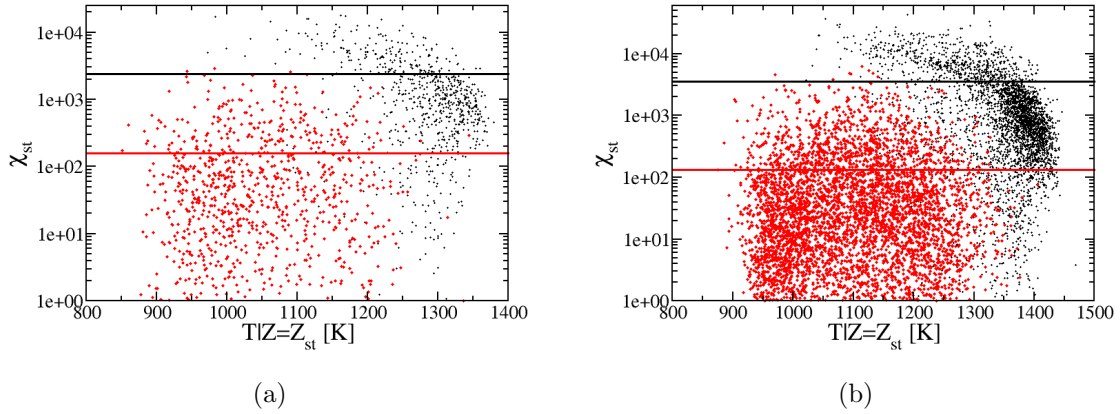
**Figure 15:** Variation of PDF of temperature,  $H_2O$  and  $OH$  mass fraction on stoichiometric plane at extinction: (a),(c),(e) and reignition: (b),(d),(f) for Case H with TANN-2

F-GRID, respectively. A very small fraction of points lie above this mean and has  $\chi_{st}$  values as high as 4 times and 8 times greater than mean  $\chi_{st}$  for C-GRID and F-GRID,





**Figure 16:** PDF of the normalized scalar dissipation rate at the stoichiometric mixture for Case H with TANN-2. (a) C-Grid, (b) F-Grid

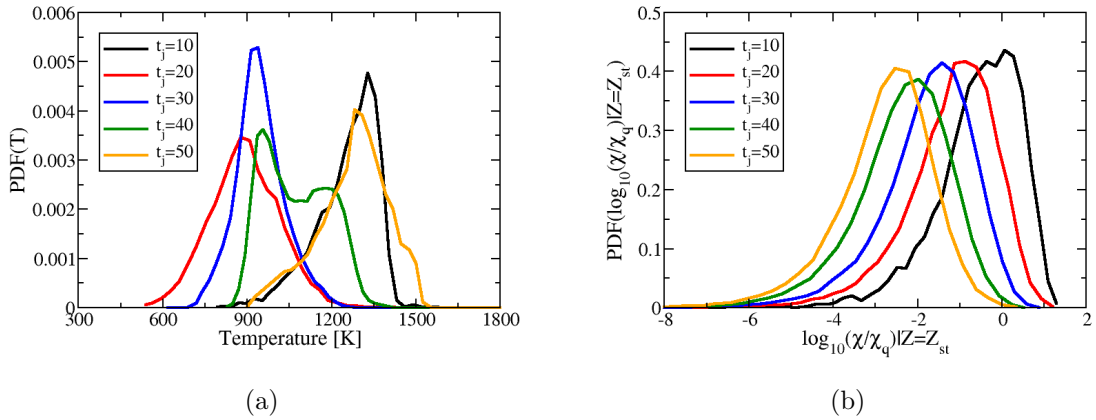


**Figure 17:** Distribution of  $\chi_{st}$  with respect to temperature on the stoichiometric plane for Case H. Black dots:  $t_j = 10$ , Red dots:  $t_j = 40$  for (a) C-GRID, (b) F-GRID

respectively. It is also observed that at extinction points with  $\chi_{st}$  values above the mean  $\chi_{st}$  lie at lower temperatures indicating the formation of extinguished regions [36]. At  $t_j = 40$  the stoichiometric data is spread over a wider range of temperature compared to the stoichiometric data at  $t_j = 10$  and it is spread more uniformly about a lower mean of  $\chi_{st}$  of 130 and 160 for C-GRID and F-GRID, respectively, which indicates partial reignition. This results in less negative skewness. Further it is observed that at  $t_j = 10$  the stoichiometric data is more clustered below  $\chi_{st} = 2000$  for

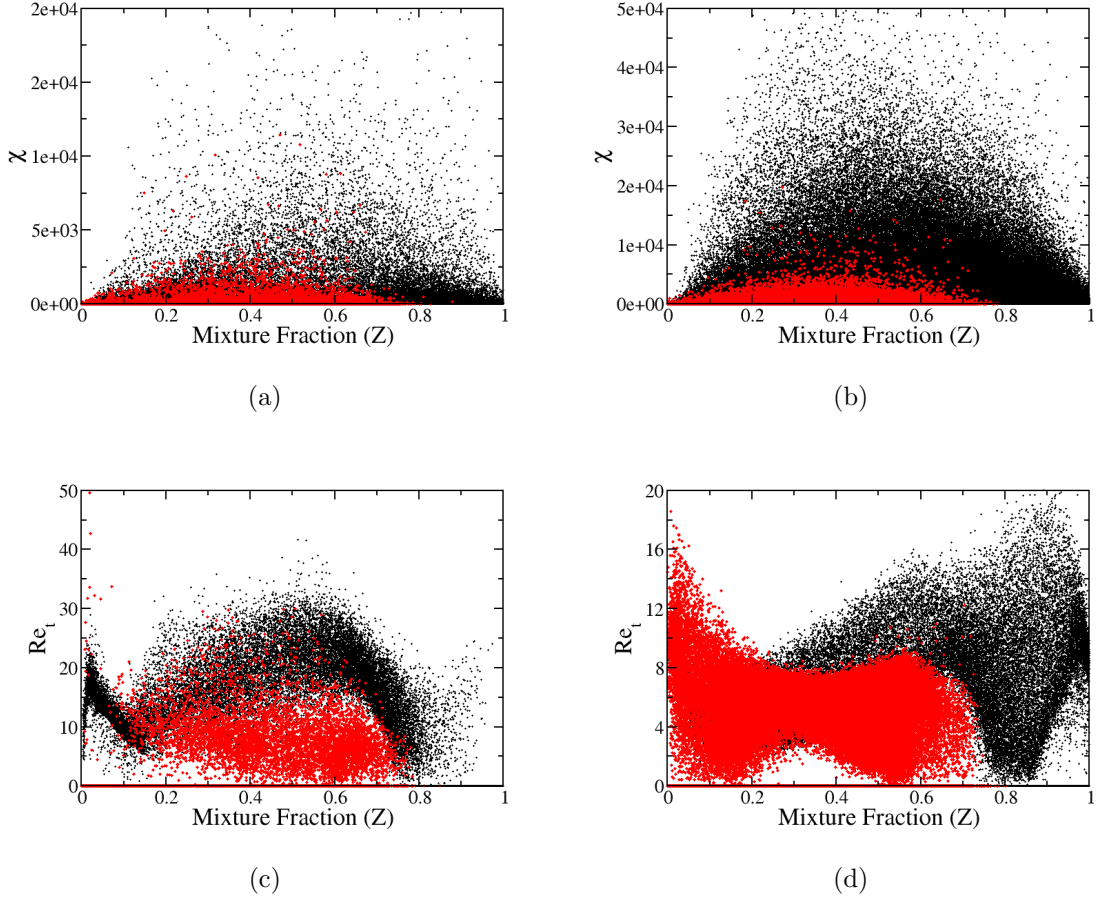
F-GRID compared to C-GRID. This has led to the smoother normalized  $\chi_{st}$  profile for F-GRID compared to C-GRID at normalized  $\chi_{st}$  values less than -3. Similar to  $t_j = 40$  at  $t_j = 20$  and  $t_j = 30$ , the mean  $\chi_{st}$  is low and hence the negative skewness is not observed. Overall, the pdf of normalized  $\chi_{st}$  for C-GRID and F-GRID are in good agreement.

Fig. 18(a) and 18(b) show the evolution of temperature and  $\chi$  pdf on stoichiometric plane with time for case H M-GRID. The temperature pdf shifts rapidly to lower mean value and the variance increases going from  $t_j = 10$  to  $t_j = 20$ . By  $t_j = 30$  the variance decreases and with further increase in time the temperature pdf shifts to higher values. The  $\chi$  pdf shifts to lower values with time. These results show that the TANN-2 is capable of capturing the complex extinction-reignition phenomenon and also handling grids of different resolutions. Fig. 19(a) and 19(b) show the  $\chi$  vs  $Z$



**Figure 18:** Evolution of the pdf on stoichiometric plane of (a)temperature and (b)scalar dissipation rate of  $Z$  for Case H M-GRID using TANN-2

data for case L and case H F-GRID, respectively, at the location of maximum mean  $\chi_{st}$  and at  $t_j = 40$ . The  $\chi$  distribution reaches much higher values for both the cases at the location of maximum mean  $\chi_{st}$  compared to the distribution at  $t_j = 40$ . The maximum  $\chi$  value observed for case L is around 20,000 where as for case H F-GRID it goes upto 50,000. Thus,  $\chi$  distribution for case L lies inside the training data space

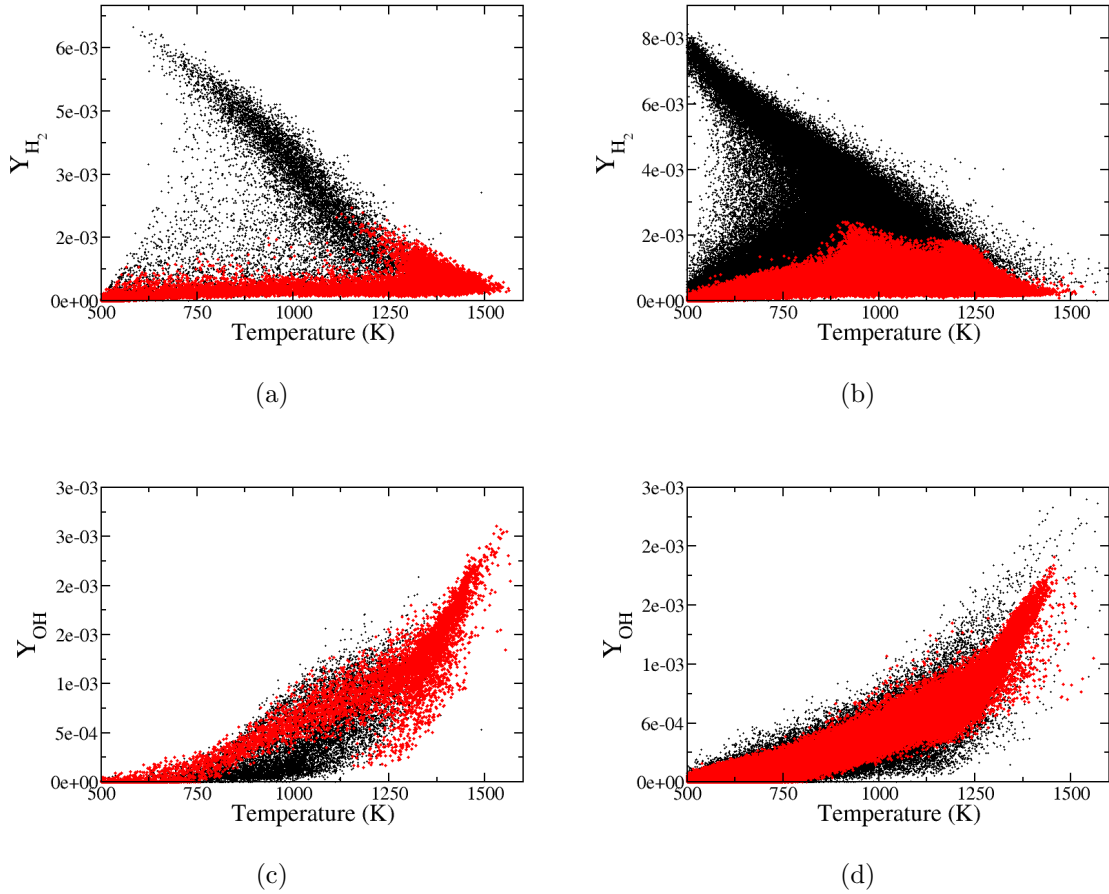


**Figure 19:** Comparison of  $\chi$  and  $Re_t$  with respect to Z. (a) and (c) represent Case L with Black symbols:  $t_j = 15$  and Red symbols:  $t_j = 40$ . (b) and (d) represent Case H F-GRID with Black symbols:  $t_j = 12$  and Red symbols:  $t_j = 40$

of both TANN-1 and TANN-2. Whereas, for case H F-GRID  $\chi$  distribution lies inside the training data space of TANN-2 only. Which is the cause of the failure of TANN-LES using TANN-1 in capturing the extinction-reignition for case H. Fig. 19(c) and 19(d) show the  $Re_t$  vs Z data for case L and case H F-GRID, respectively. Both the cases reach the higher  $Re_t$  values at the location of maximum  $\chi_{st}$  compared to  $t_j = 40$ . The maximum  $Re_t$  observed for case L and case H F-GRID are around 40 and 20, respectively. For case H F-GRID the maximum  $Re_t$  is lower because of the finer grid size used. Comparing the  $Re_t$  distribution of the two cases with  $Re_t$  distribution of TANN-1 and TANN-2 training data, it is observed that both TANN-1 and TANN-2

training data cover the  $Re_t$  data space of the two test cases.

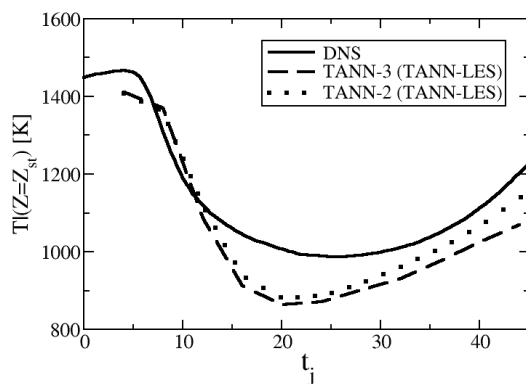
Fig. 20(a) through 20(d) show the distribution of mass fraction of  $H_2$  and  $OH$  vs temperature for case L and case H F-GRID. The thermo-chemical data space for the two cases cover similar regions at extinction or reignition. Based on the comparisons between the training data and the two test cases data, it is observed TANN-1 fails to cover only the  $\chi$  data space of case H, whereas TANN-2 covers the entire data space of both case L and case H.



**Figure 20:** Comparison of  $H_2$  and  $OH$  mass fraction with respect to temperature. (a) and (c) represent Case L with Black symbols:  $t_j = 15$  and Red symbols:  $t_j = 40$ . (b) and (d) represent Case H F-GRID with Black symbols:  $t_j = 12$  and Red symbols:  $t_j = 40$

#### 4.8 Study extinction-reignition using TANN-3 trained as a function of species dissipation rate instead of species gradient

The TANN-LES using TANN-3 net is performed for Case H with M-GRID and the results are compared with DNS and TANN-LES using TANN-2 (using species gradient instead of species scalar dissipation rates). As shown in Fig.4.8 no significant difference is observed between the two TANN-LES results.



**Figure 21:** Comparison of mean temperature variation on stoichiometric plane w.r.t. non-dimensional time for Case H M-GRID using TANN-3 and TANN-2

#### 4.9 Time Savings

The computational time required to run a single iteration per grid point on a 220 processors INTEL PC (3.2 GHz Xenon) by DI-LEMLES, LANN-LEMLES and TANN-LES for case H F-GRID are given in table 3. The TANN-LES approach provides a speed-up of 33 times compared to DI-LEMLES with reasonable accuracy, where as LANN-LEMLES provides 6.6 times, for case H.

**Table 3:** Comparison of speed-up obtained by various models

Case	Model	CPU time per step per cell	speed-up
H F-GRID	DI-LEMLES	4.95 ms	1
	LANN-LEMLES	0.75 ms	6.6
	TANN-LES	0.15 ms	33

## CHAPTER V

### CONCLUSIONS

In the present work, ANN methodology is used for multi-step finite rate kinetics within the LES framework. Unlike the previous work [34] where ANN was used as a subgrid combustion model within the LES framework (LANN-LEMLES), here ANN is used for calculating the filtered reaction rates directly within the LES framework (TANN-LES). The thermo-chemical data for training the TANN is obtained by filtering the data obtained from a 1D standalone simulation over the LES grid-size [35]. The comparison of the laminar source terms and filtered source terms for the same composition show significant difference. The filtered source terms are trained as a function of the filtered mass fraction of all the species, filtered temperature and the gradient of the species. The species are trained separately.

The TANN-LES is used to simulate the temporally evolving syngas-air diffusion flames, exhibiting significant extinction-reignition, extensively studied by DNS [14] previously. TANN-LES methodology is first validated against DI-LEMLES, LANN-LEMLES and DNS results for the low  $Re$  case. The temporal variation of the mean temperature on the stoichiometric plane from TANN-LES results compare well with the DI-LEMLES, LANN-LEMLES with significant speed-up. Comparison with DNS show lower temperature on stoichiometric plane at extinction due to addition of isotropic turbulence in shear layer along a higher thickness, in LES. To further investigate the TANN-LES approach the conditional statistics are extracted and compared with the DNS data at extinction ( $t_j = 20$ ) and reignition ( $t_j = 40$ ). It is observed that the location of the maximum mean temperature does not lie at the stoichiometric mixture fraction due to differential diffusion effects, instead it lies towards the fuel

rich side. The same trend is observed for the H<sub>2</sub>O mass fraction. A comparison of the pdf of temperature and H<sub>2</sub>O mass fraction indicate slight under prediction of reignition by TANN-LES. Overall, the TANN-LES predictions match well with LEMLES predictions.

The low  $Re$  case specific TANN fails to capture the extinction-reignition phenomenon for the high  $Re$  case. An attempt is made in generalizing the TANN approach by generating a TANN that can simulate cases with different  $Re$  and grid resolutions. The training table for the "generalized" net is generated by running the standalone LEM simulation for a large range of  $Re_t$  and an intermediate filter-size. The TANN-LES results using the generalized net obtained for the high  $Re$  case with three different grid resolutions compare well with the DNS data, showing grid independence and capability of the generalized net in handling different grid resolutions. Both coarse grid and the fine grid capture the negative-skewness at high scalar dissipation rate in the pdf of the normalized scalar dissipation rate. Comparison of the TANN-LES results for the low  $Re$  case using the generalized net with the TANN-LES results using the case specific net show that loss in accuracy by the use of the generalized net is negligible.

A comparison of the training data for the two TANNs with the data from the two  $Re$  cases show that both the nets cover the same compositional data space and the thermochemical data from the LES forms a subset of the thermochemical data space of the nets. The  $\chi$  and the  $Re_t$  data space explored by the two nets differ. The  $Re_t$  data space of the LES still forms a subset of the training data of the two nets. However, the  $\chi$  data space of the high  $Re$  case falls outside the training data space of the first net which leads to its failure in simulating the high  $Re$  case. The  $\chi$  data space for both  $Re$  cases form a subset of the  $\chi$  data space of the generalized net training data space and hence it is capable of simulating different  $Re$  cases. Hence, the current study shows that it is possible to generate a TANN capable of handling

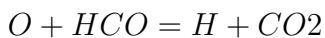
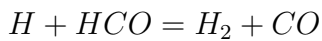
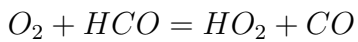
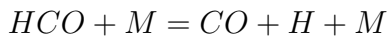
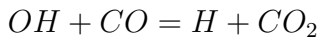
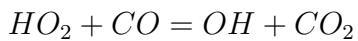
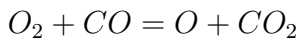
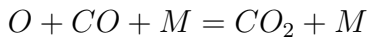
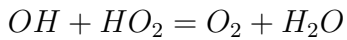
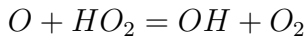
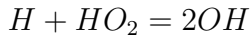
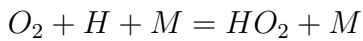
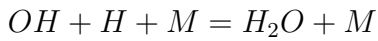
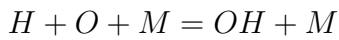
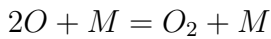
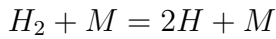
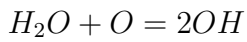
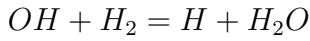
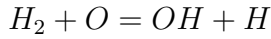
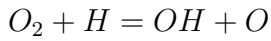


a range of  $Re$ . Thus, every new case does not require generation of a new TANN, saving significant time.

To improve the TANN methodology in future, the way of calculating  $Re_\Delta$  in the 1D standalone LEM code should be explored further. Possibly a  $k^{sgs}$ -based  $u'$  and LES  $\Delta$  can be correlated to the LEM  $u'$  and the integral length.

# APPENDIX A: 21 STEP 11 SPECIES REDUCED SYNGAS MECHANISM

Species:  $H_2$ ,  $O_2$ ,  $OH$ ,  $H_2O$ ,  $O$ ,  $H$ ,  $HO_2$ ,  $CO$ ,  $CO_2$ ,  $HCO$ ,  $N_2$



## APPENDIX B: TANN COEFFICIENTS

The TANNs generated in the present study have 14 PEs in the input layer. 10, 8 and 4 PEs in the three hidden layers. 1 PE in the output layer, since each species is trained independently. Therefore, the output of ANN training generates ten ANN coefficient tables for the ten reacting species (eleventh species is  $N_2$ ). Each PE in a given layer transmits signal to all the PEs belonging to layers downstream. The PEs in a given layer do not communicate amongst themselves. This kind of ANN architecture is called an acyclic. Therefore the total number of weight coefficients and biases written in every ANN coefficient table is:

$$\begin{aligned}
 & (\text{PEs in input layer}) \times (\sum_{n=1}^{n=3} (\text{PEs in nth hidden layer}) + (\text{PEs in output layer})) \\
 & + (\text{PEs in 1st hidden layer}) \times (\sum_{n=2}^{n=3} (\text{PEs in nth hidden layer}) + (\text{PEs in output layer})) \\
 & + (\text{PEs in 2nd hidden layer}) \times ((\text{PEs in nth hidden layer}) + (\text{PEs in output layer})) \\
 & + (\text{PEs in 3rd hidden layer}) \times (\text{PEs in output layer}) \\
 & + (\text{Sum of PEs in all the layers (bias)})
 \end{aligned}$$

$$\text{Weight connectors} = 14(10 + 8 + 3 + 1) + 10(8 + 3 + 1) + 8(3 + 1) + 3(1) = 496$$

$$\text{Biases} = (14 + 10 + 8 + 3 + 1) = 37$$

$$\text{Sum of weight connectors and biases} = 496 + 37 = 533$$

Hence, total number of values tabulated in each TANN coefficient table is 533. Note that bias of PEs in input layer is zero because the PEs in the input layer receive the full strength of the incoming signal.

Another output of the ANN methodology is the normalizing coefficients of the inputs and de-normalizing coefficients of the outputs. The values of every input in the training table are normalized between -1 to +1, corresponding to minimum and the

maximum input value, respectively. The function used is:

$$\text{Normalized}(\widetilde{Y}_{H_2}) = A_{H_2} \times \widetilde{Y}_{H_2} + B_{H_2}$$

Normalized( $\widetilde{Y}_{H_2}$ ) is the signal transmitted by the PE corresponding to  $\widetilde{Y}_{H_2}$  mass fraction in the input layer. Normalizing coefficients A and B are calculated for all the inputs using the same function. The output, source terms in the present study are normalized between -0.8 to +0.8. The source terms are normalized between -0.8 to +0.8, instead of -1 to +1 because the outgoing signal of a PE is obtained by applying hyperbolic tangent function to signal recieved. Therefore, values of -1 and +1 will require the output PE to recieve a signal of strength - and +, respectively. The output of the ANN interpolation for computing source term of  $H_2$  (ANN( $H_2$ )) is de-normalized using the function:

$$\frac{\overline{\omega}_{H_2}}{\overline{\rho}} = \frac{e^{\text{ANN}(H_2)} - D_{H_2}}{C_{H_2}}$$

Thus, a table is created in which A and B values corresponding to all inputs, and C and D values corresponding to all outputs are tabulated.

The ANN training gives 10 ANN coefficient files corresponding to each of the 10 reacting species. Each file contains 533 values. An additional table ANN.dat is created which contains the As and Bs corresponding to all inputs, and Cs and Ds corresponding to all outputs.

ANN.dat format				Sample ANN Coefficient table for a species
$A_{H_2}$	$B_{H_2}$	$C_{H_2}$	$D_{H_2}$	-3.835612931767081E-002
=	=	=	=	-0.108052176485972
=	=	=	=	-0.436501419823321
$A_{N_2}$	$B_{N_2}$	0.0	0.0	0.143977788550831
$A_T$	$B_T$	0.0	0.0	5.040344446165773E-003
$A_{Re\Delta}$	$B_{Re\Delta}$	0.0	0.0	9.986534201938069E-003
$A_{\nabla Y_{H_2}}$	$B_{\nabla Y_{H_2}}$	0.0	0.0	-0.108150477215085
=	=	=	=	=
=	=	=	=	=
$A_{\nabla Y_{N_2}}$	$B_{\nabla Y_{N_2}}$	0.0	0.0	=

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