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An RCCE-ANN Tabulation Approach Applied to Sydney Flame L

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Introduction

In order to develop more efficient and environmental friendly combustion engines comprehensive CFD simulations have to be performed. Such simulations are extremelly time demanding since they involve:

- Turbulence-chemistry interaction models (i.e. PDF).
- Chemical mechanisms with hundreds of species and thousands of reactions.
- Wide range of time and lenght scales.

Therefore, chemical step CPU time consumption must be reduced!!

Replace the production/destruction rate term

Our goal is to replace the source term by a series of polynomials through non-linear regression.

$$\dot{\omega} = \frac{\partial \phi}{\partial t} = f(x_1, ..., x_k; w_1, ..., w_n) \tag{1}$$

where

- ϕ Reactive scalar.
- x_k The k_{th} input.
- w_n The n_{th} polynomial constant.

ANN Tabulation framework

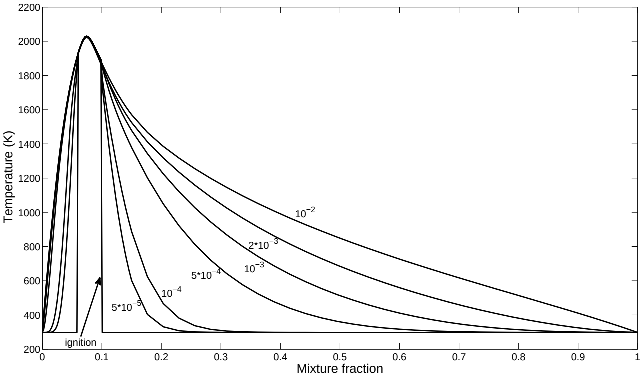
- Mechanism Reduction.
- Sample generating.
- Sample clustering.
- ANN training.
- Validation.
- Application.

Mechanism Reduction via Rate-Controlled Constrained Equilibrium (RCCE)

- Reduced mechanism framework.
- Kinetically constrained: Solved directly from the kinetics of the detailed mechanism.
- Equilibrated: Assumed to be in a constrained equilibrium.
- Kinetically constrained species from GRI 1.2: H_2O, CO_2, CH_4, CO, O_2, H_2, C_2H_2, C_2H_4,CH_3, C_2H_6, OH, O, CH_2O, CH_2CO, CH_3OH and H.

Sample generating data via ignited flamelet

- Varying strain rate from $1s^{-1}$ to $1100s^{-1}$.
- Randomly selected mixture fraction points.
- Store information of enthalpy alongside with kinetically constrained species before and after the reaction step.



Sample clustering via Self-Organazing Maps (SOM)

- Cluster the data according the their similarity.
- Preserves the probability density of the input space.
- Preserves the topology of the input space

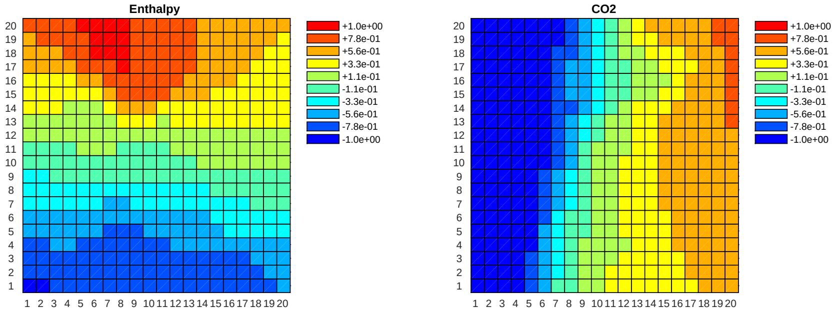


Figure: SOM map for Enthalpy and CO_2

ANN training via Multilayer Perceptron (MLP) - I

- The MLP is a non-linear mapping between two sets of variables.
- It is formed by a composition of non-linear functions.
- It involves a number of unknown coefficients, called weights (w_{ij}), to be determined by fitting pairs of input-output training data.

$$y_k = f(\sum w_{jk} y_j) \quad (2)$$

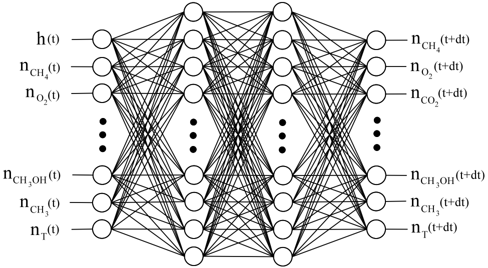


Figure: MLP topology

ANN training via Multilayer Perceptron (MLP) - II

- In order to adjust the weights (w_{ij}) the conjugate gradient optimzation technique is employed.
- It is performed by the minimization of the mean square error

$$E_k = \frac{1}{2}|y_k - y_{true}|^2 \tag{3}$$

$$f(...) = min(E_k) \tag{4}$$

where

- E_k Cost function.
- y_k Prediction given by the MLP.
- y_{true} RCCE output value.

Validation with unseen data

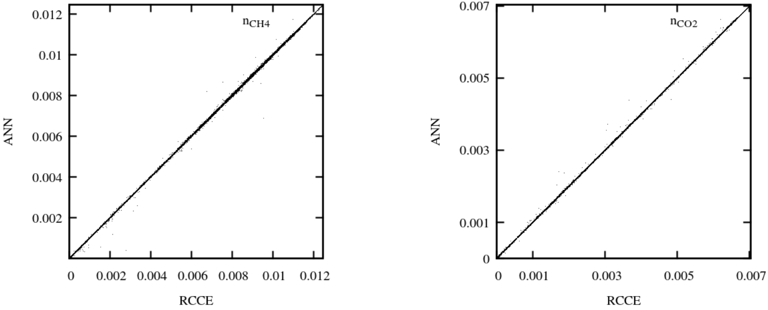


Figure: Comparison of unseen data points ANN prediction against the RCCE target values

$$\text{Mean}_{RMS} = 0.836\text{E-}6$$

Application to turbulent non-premixed Sydney L flame

Simulations performed in the in-house BOFFIN-LES:

- LES of a variable density flow advecting a number of reactive scalars.
- The turbulence-chemistry interaction is closed by the PDF method.
- For turbulent transport, we adopt a Smagorinsky model.
- A cartesian grid comprising 360x96x96 points is employed.
- The Eulerian stochastic fields method comprising 8 fields is applied as the solution scheme.
- Simulations are performed on the ARCHER UK National Supercomputing Service, employing 80 processors.

Sydney Flame L

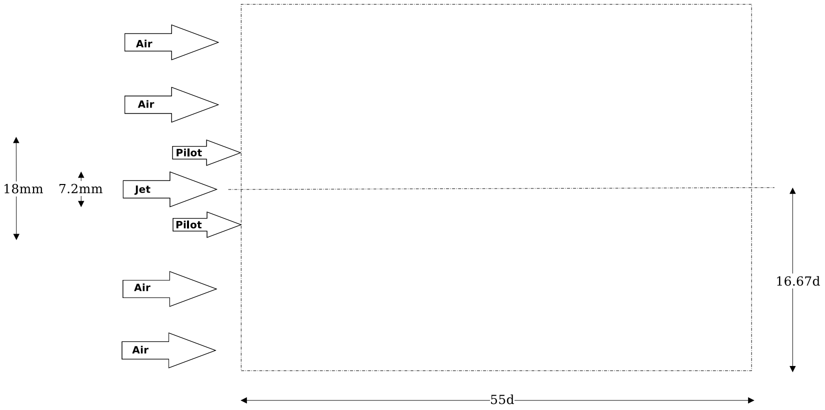


Figure: Schematic representation of the flow domain for the Sydney flame L

Mean Fields - I

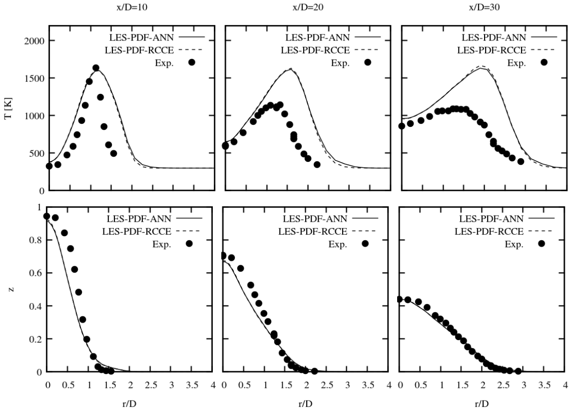


Figure: LES-PDF-ANN and LES-PDF-RCCE mean temperature and mixture fraction radial profiles

Mean Fields - II

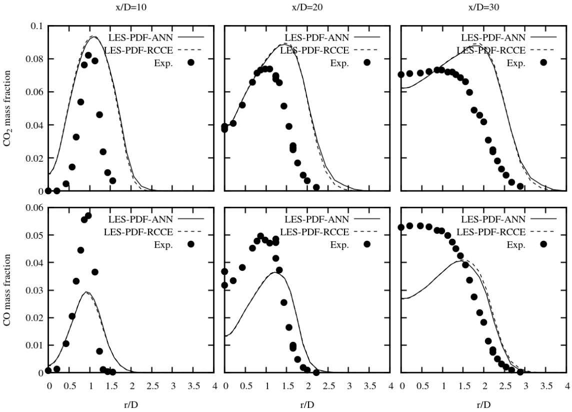


Figure: LES-PDF-ANN and LES-PDF-RCCE mean CO_2 and CO mass fraction radial profiles

RMS Fields - I

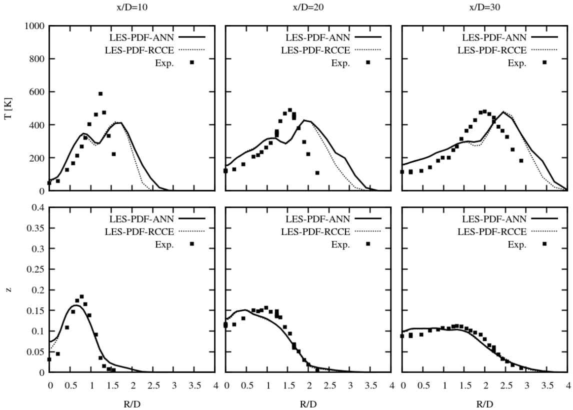


Figure: LES-PDF-ANN and LES-PDF-RCCE rms temperature and mixture fraction radial profiles

RMS Fields - II

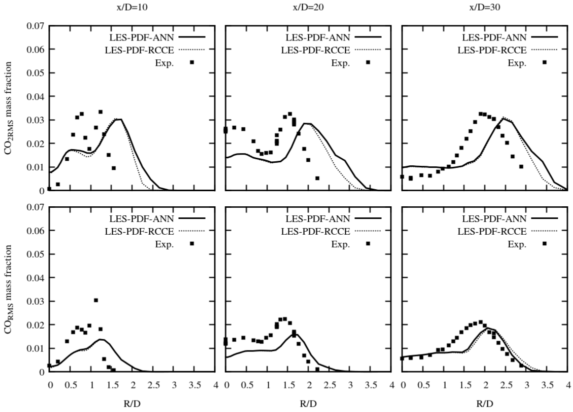


Figure: LES-PDF-ANN and LES-PDF-RCCE mean CO_2 and CO mass fraction radial profiles

Time measurement and storage space

Method	Convection-Diffusion (s)	Reaction (s)
RCCE	7	125
ANN	7	1.5

Table: Average CPU time for ANN and RCCE real time integrator

Finally, the disk storage space required for the ANNs (i.e. the weights) is only 36 MB!

Concluding remarks

Advantages of the RCCE-ANN tabulation framework:

- Easy to implement (or to combine with existing software).
- Accurately reproduces the mean and rms profiles given by the reduced mechanism (RCCE).
- Reduced the computational cost by two orders of magnitude compared to the reduced mechanism (RCCE).
- Very small disk storage space requirement.

Acknowledgement

CNPq
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Thank you very much