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Tabulation of Combustion Chemistry via Artificial Neural Networks

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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 non-linear regression process.

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

where

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

ANN Tabulation framework

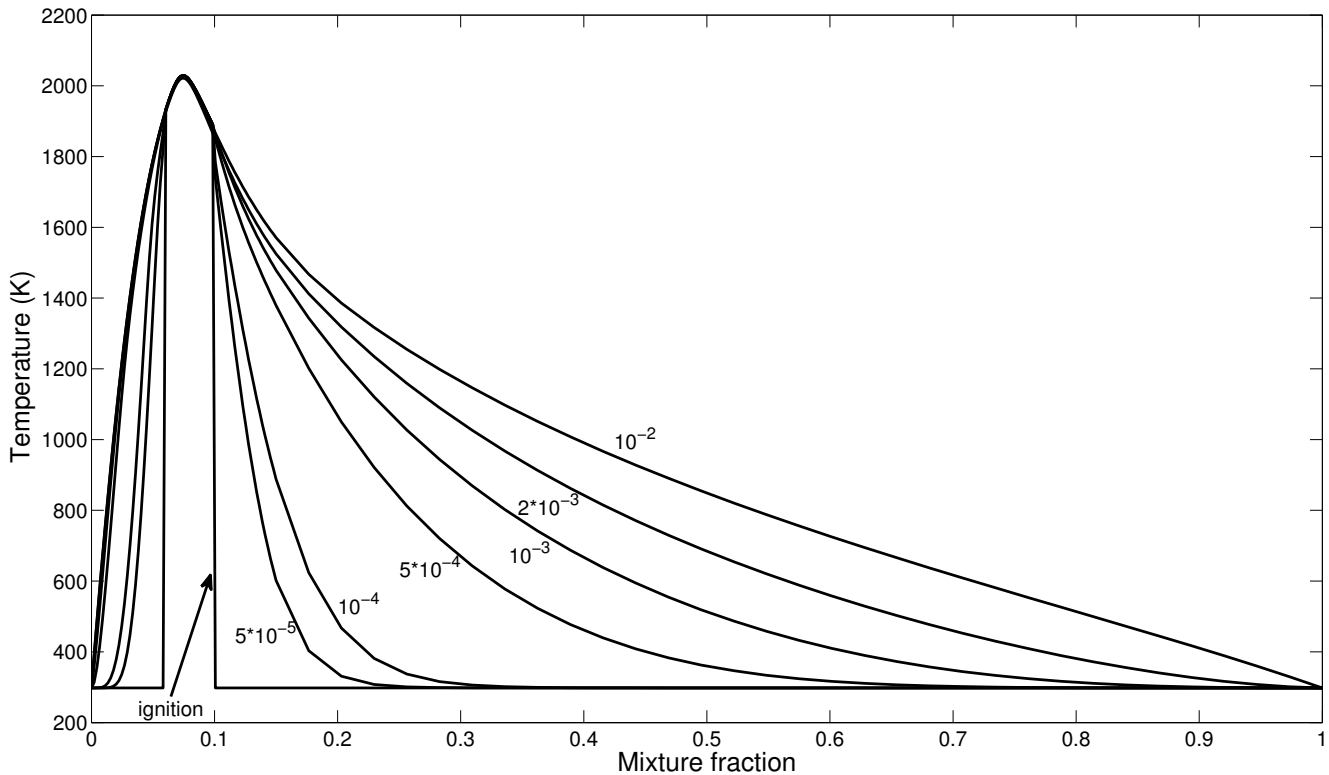
- Mechanism Reduction.
- Sample generating.
- ANN training.
- Validation.
- Application.

1 - 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.

2 - Sample generating data via ignited flamelet

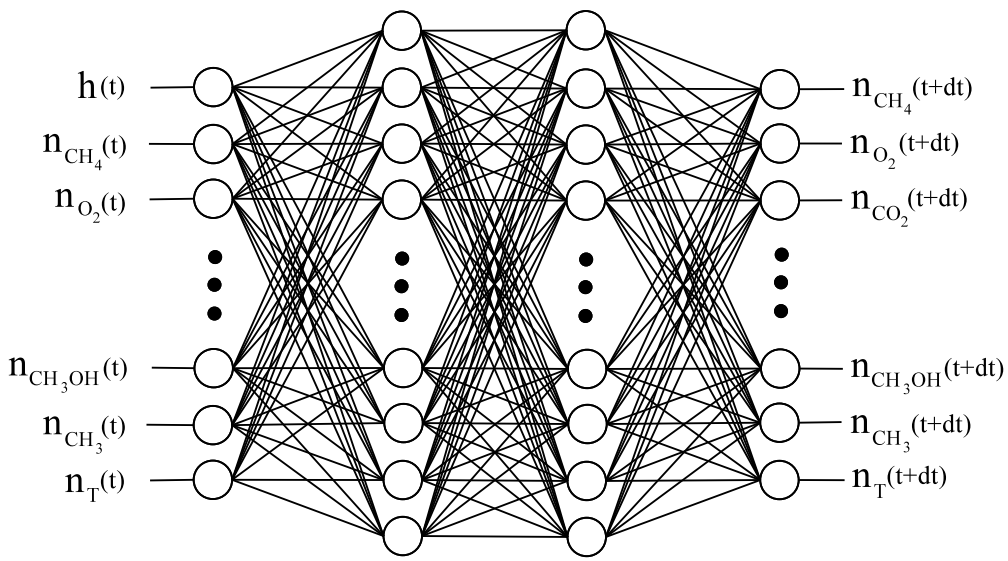
- Varying strain rate from $1s^{-1}$ to $1100s^{-1}$.
- Randomly selected mixture fraction points.
- Store information of enthalpy alongside with kinetically constrained species before and after the reaction step.



3 - ANN training

- The ANN is a non-linear mapping between two sets of variables.
- It involves a number of unknown coefficients, called weights (w_{ij}), to be determined by a training step following the pairs of input-output data.
- Training is performed by conjugate gradient optimization, minimizing the mean square error between $\text{ANN}_{outputs}$ and $\text{RCCE}_{outputs}$.

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



4 - Validation with unseen data

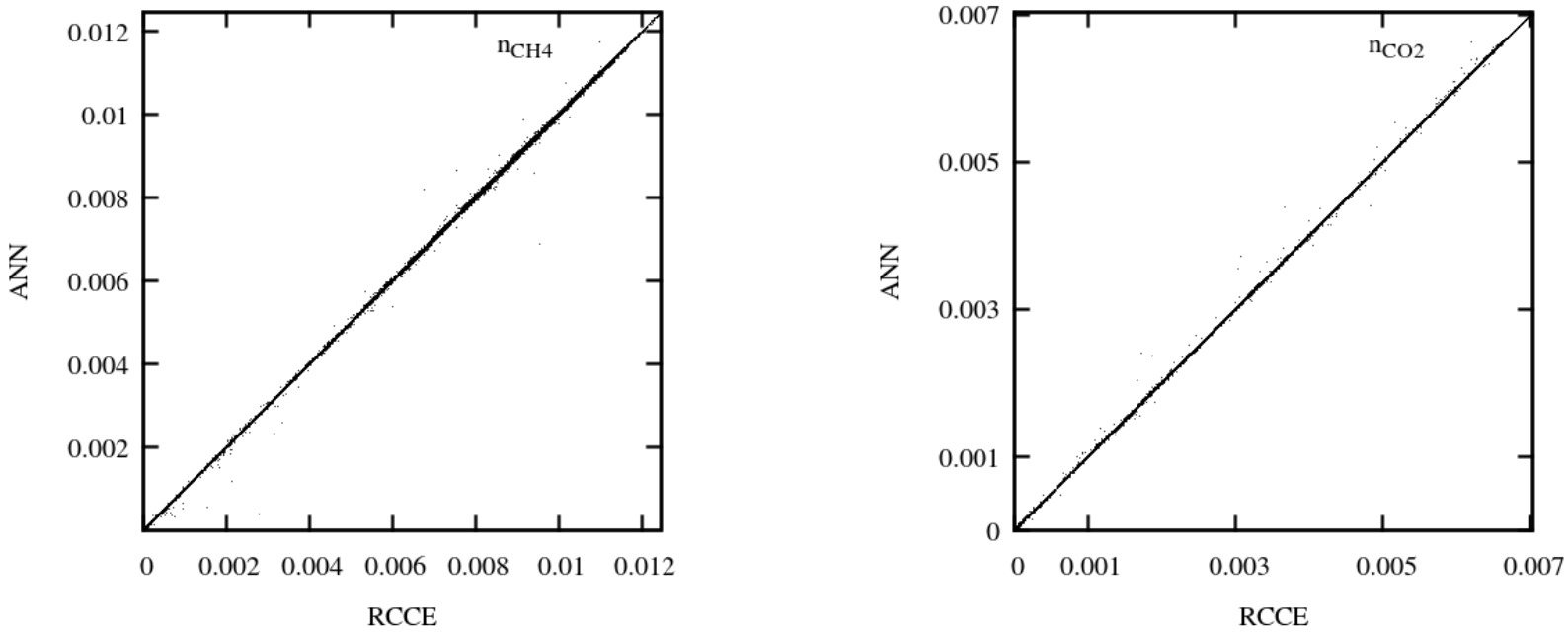


Figure: Comparison of unseen data points ANN prediction against the RCCE target values

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

5 - Application to turbulent non-premixed flame

We consider a combined LES-PDF model:

- LES of a variable density flow advecting a number of reactive scalars.
- The turbulence-chemistry interaction is closed by the PDF method.
- The Eulerian stochastic fields method comprising 8 fields is applied as the solution scheme via the Monte Carlo estimator.

$$\rho\partial\xi_\alpha^n = -\rho\tilde{u}\frac{\partial\xi_\alpha^n}{\partial x}dt + \rho\dot{\omega}(\phi)\xi_\alpha^n dt + \frac{\partial}{\partial x}[(\frac{\mu}{\sigma} + \frac{\mu_{sgs}}{\sigma_{sgs}})\frac{\partial\xi_\alpha^n}{\partial x}]dt - \frac{\rho}{2\zeta_{sgs}}[\xi_\alpha^n - \tilde{\phi}]dt + \sqrt{2\rho\Gamma}\frac{d\xi_\alpha^n}{dx}dW \tag{3}$$

$$\tilde{\phi}_\alpha = \frac{1}{N}\sum_{n=1}^{N}\xi_\alpha^n \tag{4}$$

- Simulations are performed on the ARCHER UK National Supercomputing Service, employing 80 processors.

Sydney Flame L

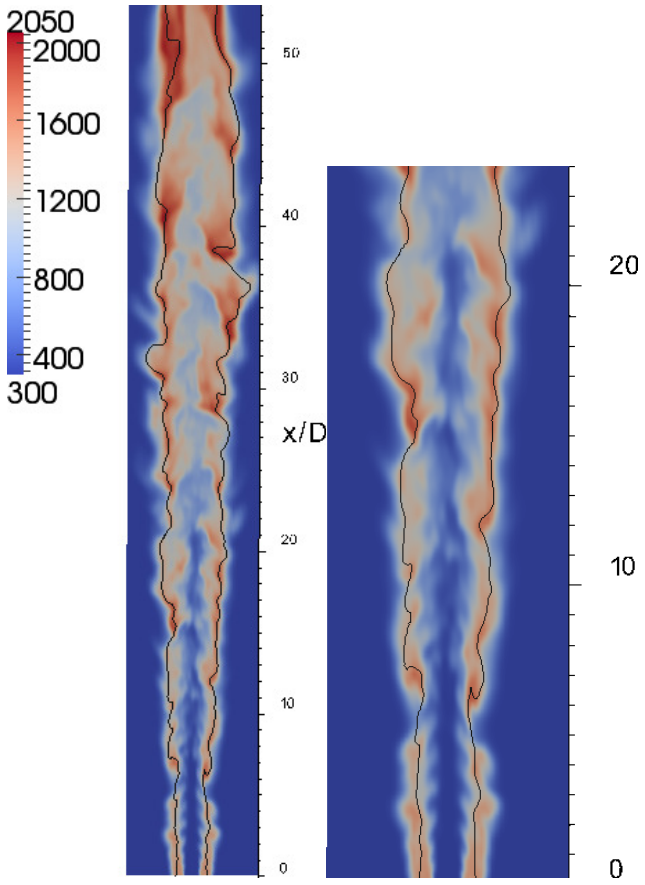


Figure: Contour plots of Sydney flame L computed with LES-PDF-ANN: a) full domain b) zoom on the middle section of the flame.

Results presented in the Combustion and Flame Journal Paper: Tabulation of Combustion Chemistry via Artificial Neural Networks (ANNs): Methodology and Application to LES-PDF Simulation of Sydney Flame L

Mean Fields - I

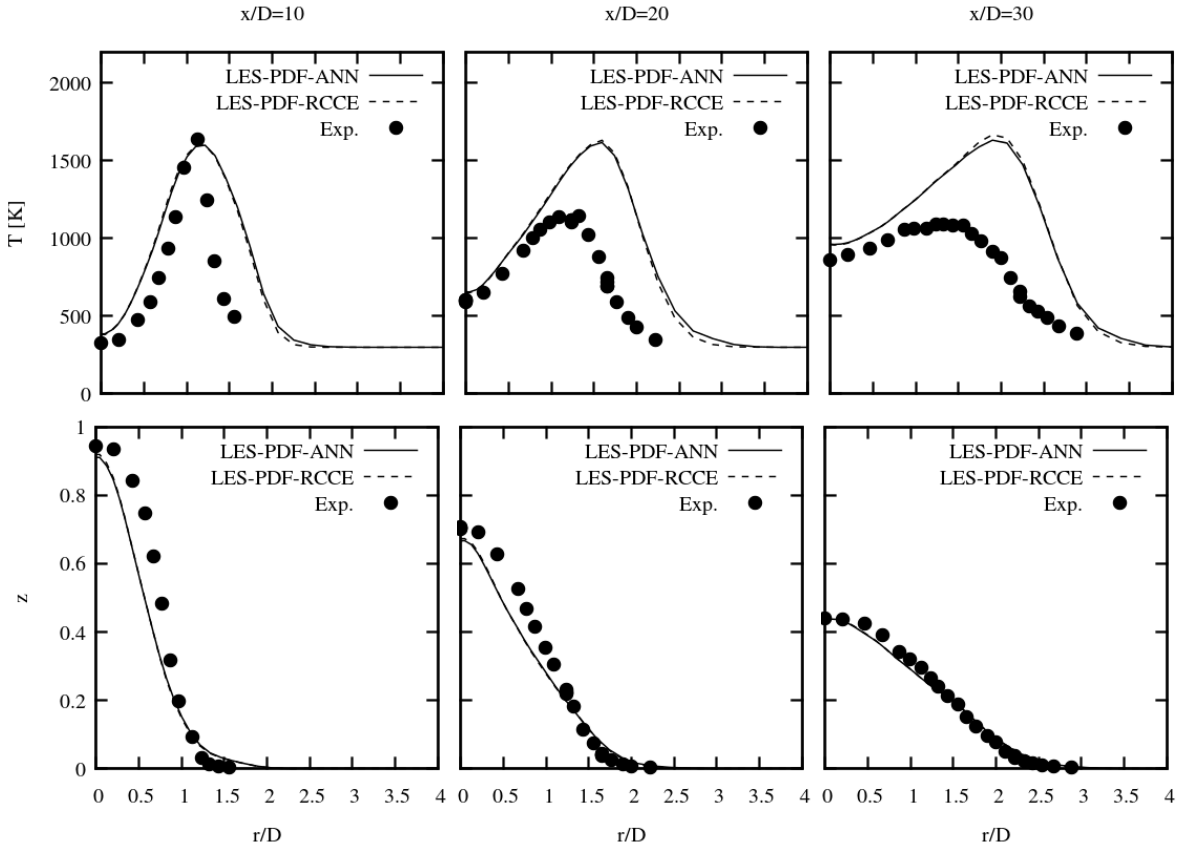


Figure: LES-PDF-ANN and LES-PDF-RCCE mean temperature and mixture fraction radial profiles

Results presented in the Combustion and Flame Journal Paper: Tabulation of Combustion Chemistry via Artificial Neural Networks (ANNs): Methodology and Application to LES-PDF Simulation of Sydney Flame L

Mean Fields - II

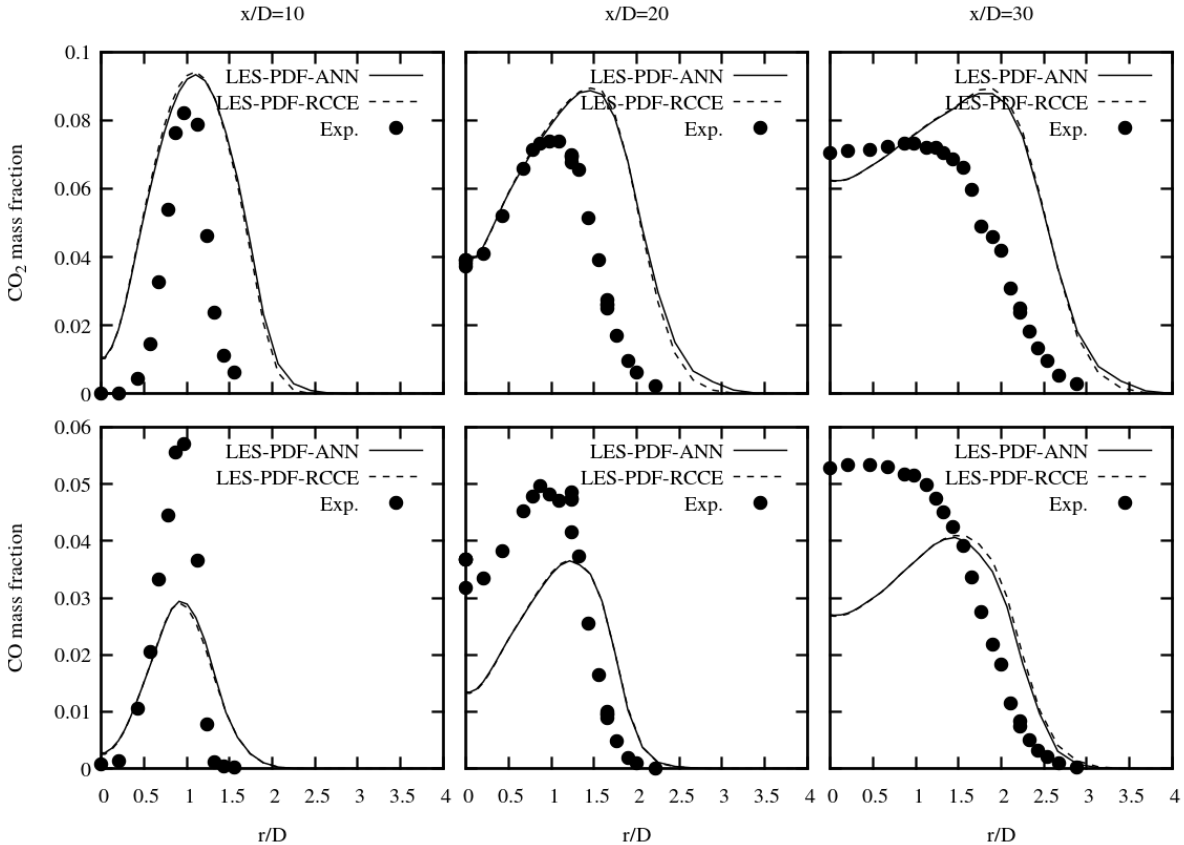


Figure: LES-PDF-ANN and LES-PDF-RCCE mean CO_2 and CO mass fraction radial profiles

Results presented in the Combustion and Flame Journal Paper: Tabulation of Combustion Chemistry via Artificial Neural Networks (ANNs): Methodology and Application to LES-PDF Simulation of Sydney Flame L

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.

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Thank you very much