# *Automatic Generation of Networks for Emissions Simulation*

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# Combustion in Aviation

- Gas turbine engines for propulsion
- Energy conversion by combustion of fuel to produce thrust.
- Advisory Council for Aviation Research and Innovation in Europe (ACARE) regulations on CO2, CO, NOx emissions[1].


Source: https://blog.klm.com/as-fit-as-a-jet-engine/

1] Flight Path 2050 and ACARE Goals for Maintaining and Extending Industrial Leadership in Aviation: A Map of the Aviation Technology Space, Sustainability 2019, 11, 2065; doi:10.3390/su11072065

# *Combustion Modelling*

- Computational Fluid Dynamics(CFD): Turbulence modelling+ Chemistry modelling

- Most often: reduced chemistry model

- Emissions such as CO and NOx dependent on intermediate species and radical concentrations and are typically slower than reactions responsible for heat release.

  - Hence detailed chemical mechanism required.

- Too expensive to include in CFD

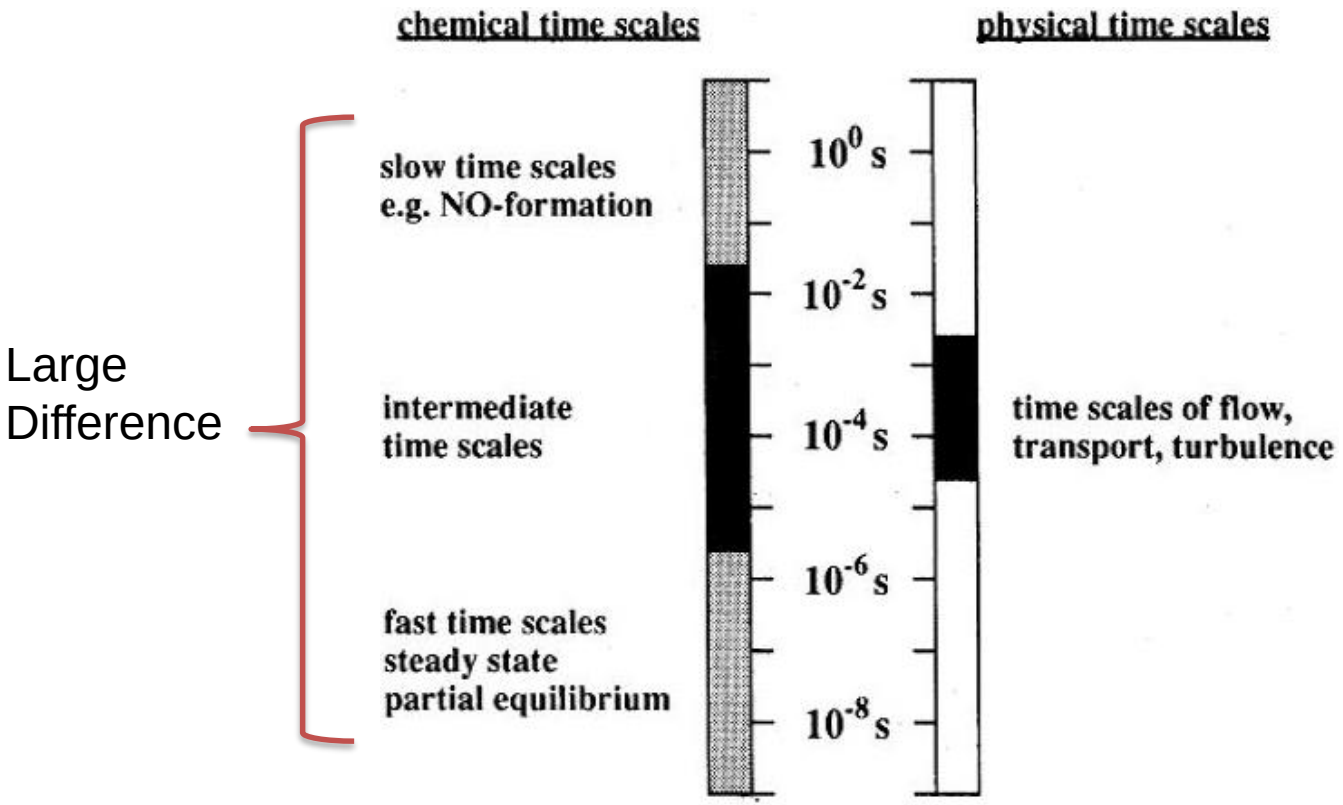
# *Combustion Chemistry*

- Non-linear
- Stiffness

# Non-linearity

- For reaction : $mA + nB \rightarrow pC + qD$
  - $-\frac{1}{m}\frac{d[A]}{dt} = k[A]^m[B]^n$
  - Where, $k = Ke^{-\frac{E_a}{RT}}$
- Power Law
- Exponential dependence on temperature

# Stiffness


chemical time scales
physical time scales
Large
Difference
slow time scales
e.g. NO-formation
intermediate
time scales
fast time scales
steady state
partial equilibrium
$10^{0}$ s
$10^{-2}$ s
$10^{-4}$ s
$10^{-6}$ s
$10^{-8}$ s
time scales of flow,
transport, turbulence

# CFD-CRN

- Decouple fluid mechanics and chemistry calculation
  - Step1: CFD with minimal chemistry to account for heat release.
  - Step2: Chemical Reactor Network to account for detailed chemistry.
- Assumption: Minor species, do not contribute much to energy release and hence have a small influence on the flow field.

[2] Stagni et al, Computer and Chemical Engineering 60(2014) 197-212
[3] M. Falcitelli, L. Tognotti, and S. Pasini, An algorithm for extracting chemical reactor network models from cfd simulation of industrial combustion systems, Combustion Science and Technology **174**, 27 (2002).

# Chemical Reactor Network

- PSR(Perfectly stirred reactor):
  - 0D ideal reactor model
  - homogeneously mixed
- Network of PSRs
- CRN: Mass, Species and Energy equations
- 0D leads to a system of ODEs

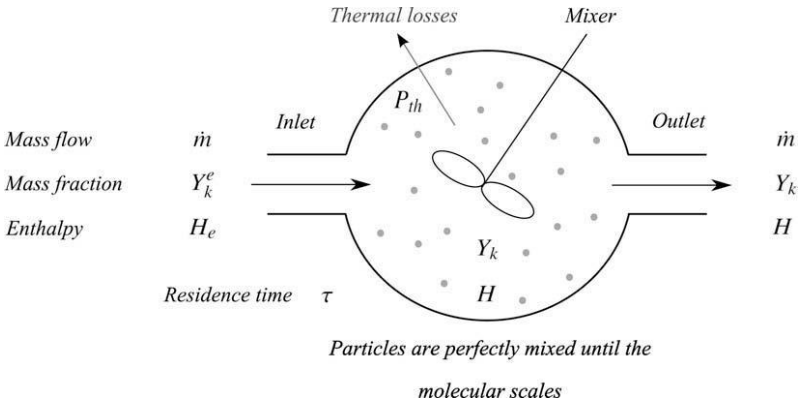



**Fig: PSR representation**

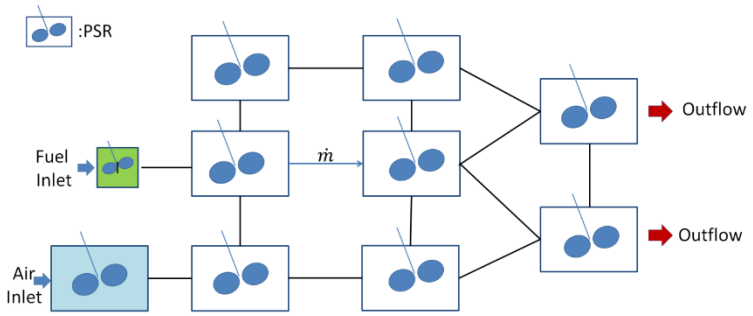



**Fig: CRN representation**

# Chemical Reactor Network

- $g(\omega) = m\frac{d\omega}{dt} = \sum_{in} \dot{m}_{in}(\omega_{in} - \omega) + V\dot{\omega}(MW)$
- Equation for 1 species in 1 reactor
- System of equations of $N_S$ species and $N_R$ reactors.
- Solve for steady state: $g(\omega) = 0$

# AGNES

- Software tool developed in Python to implement CFD-CRN process.
- Automatically generate CRN from CFD solution without explicit partitioning
- Cantera[4] used for chemistry bookkeeping
- Clustering->Solver

[4] David G. Goodwin, Raymond L. Speth, Harry K. Moffat, and Bryan W. Weber. *Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes*. https://www.cantera.org, 2018. Version 2.4.0. doi:10.5281/zenodo.1174508

# Clustering

- Reducing 1e^6 CFD cells to 1e^3 reactors.
- Each reactor deals with ~(53-100) chemical species.
- Clustering done based on user defined criteria: Eg - Temperature, Mass fraction of $O_2$, Mass fraction of $CH_4$

- Breadth First Search method
  - Traverse through children at same level first
  - Ensures that clustered cells are similar and physically connected

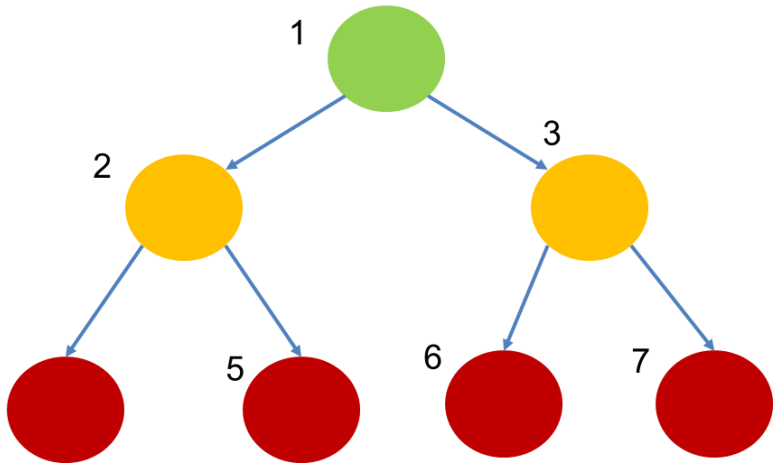



Fig: BFS algorithm

# Clustering

- Mass flow exchange between reactors based on CFD result.

- Initial thermodynamic and chemical state of reactors based on weighted average of agglomerated cells.

- Mass Balance recalculated based on ratio of mass flow exchanged with neighbouring reactor and total inflow into a reactor.

  - CFD solution will have some convergence tolerance and this adds up during clustering.

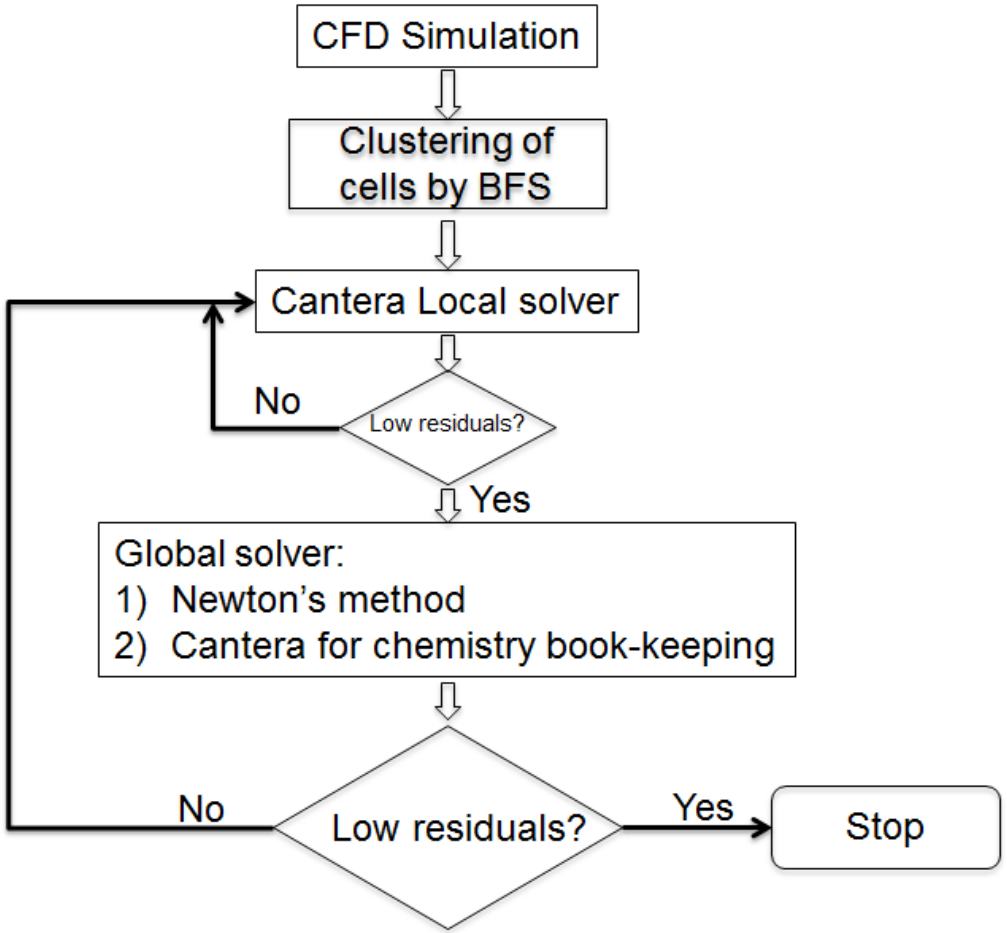
$$M_k - \sum_{j \neq k}^{N} \alpha_{kj} M_j = \sum f_k$$

$$\begin{bmatrix} \alpha_{11} & -\alpha_{12} & -\alpha_{13} & -\alpha_{14} & .. & .. \\ -\alpha_{21} & \alpha_{22} & -\alpha_{23} & .. & .. & .. \\ -\alpha_{31} & -\alpha_{32} & \alpha_{33} & .. & .. & .. \\ : & : & : & .. & .. & .. \end{bmatrix} \begin{bmatrix} M_1 \\ M_2 \\ : \\ : \end{bmatrix} = \begin{bmatrix} \sum f_1 \\ \sum f_2 \\ : \\ : \end{bmatrix}$$

# *Solver*

- Local Solver: solve individual reactors while considering the rest constant. Subsequent iterations over all reactors.
  - Cantera's Reactor Network solver used.
- Global Solver:
  - Larger system of equations ~ $N_S$ x $N_R$
  - Newton Solver: fast gradient based stepping towards steady state solution
  - Pseudo Time-stepping: BDF, for when Newton's method diverges.

# AGNES flowchart



# Test Case

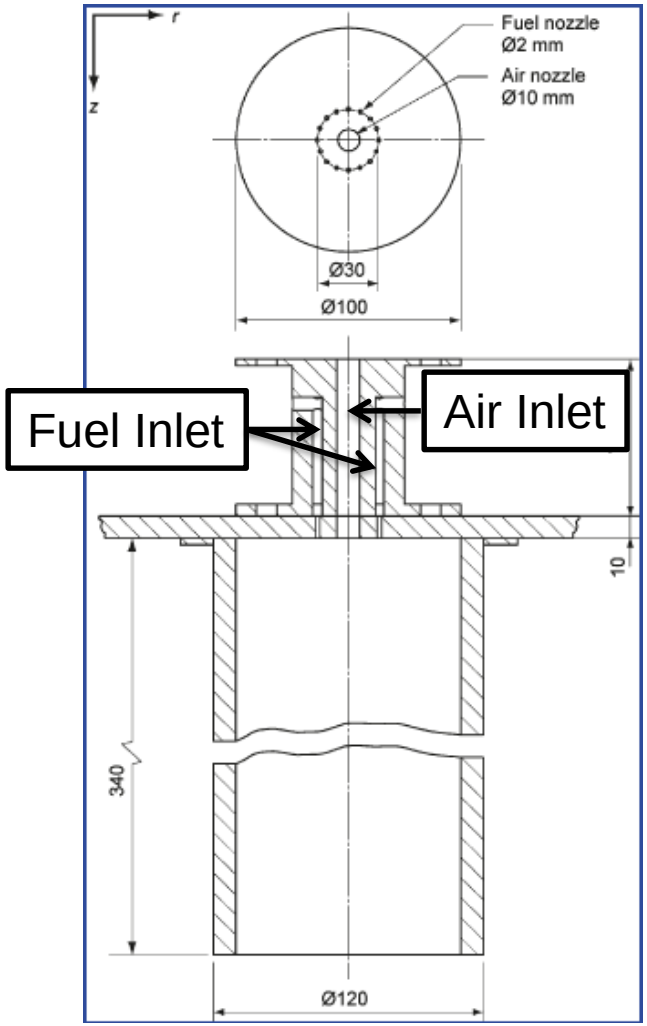



**Fig: Schematic of Combustor**

Fuel: Methane(CH4) @ 300K
Oxidizer: Air @ 673K

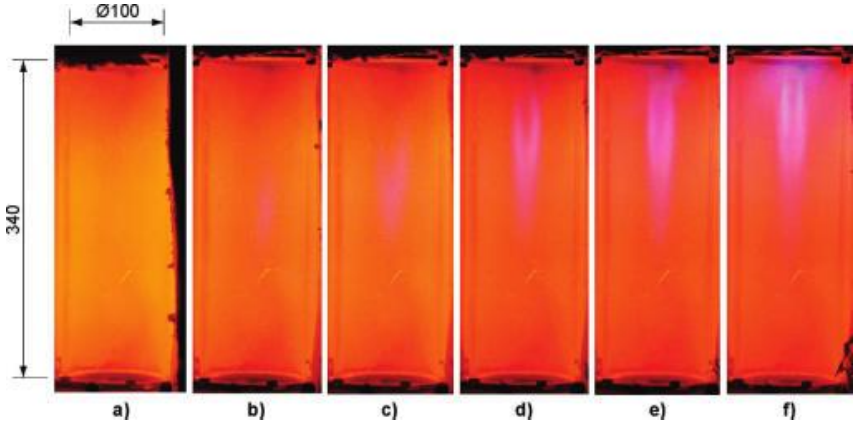
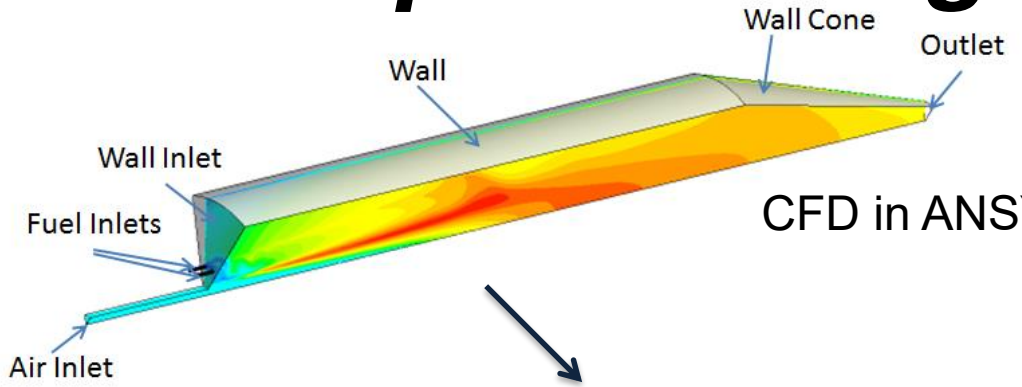



**Fig: Appearance of combustion modes**

[5] A. S. Veríssimo, A. M. A. Rocha, and M. Costa, Operational, Combustion, and Emission Characteristics of a Small-Scale Combustor, Energy Fuels 2011, 25, 2469–2480

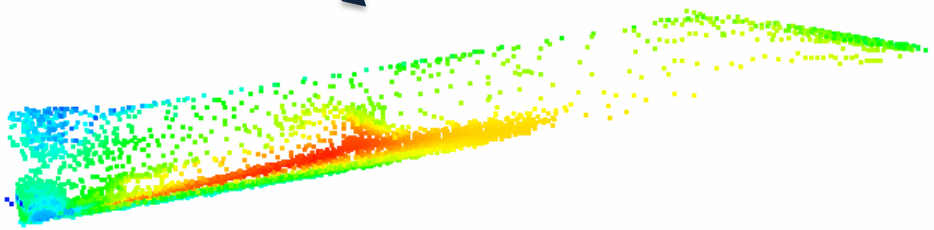
# AGNES processing




CFD in ANSYS Fluent™

AGNES

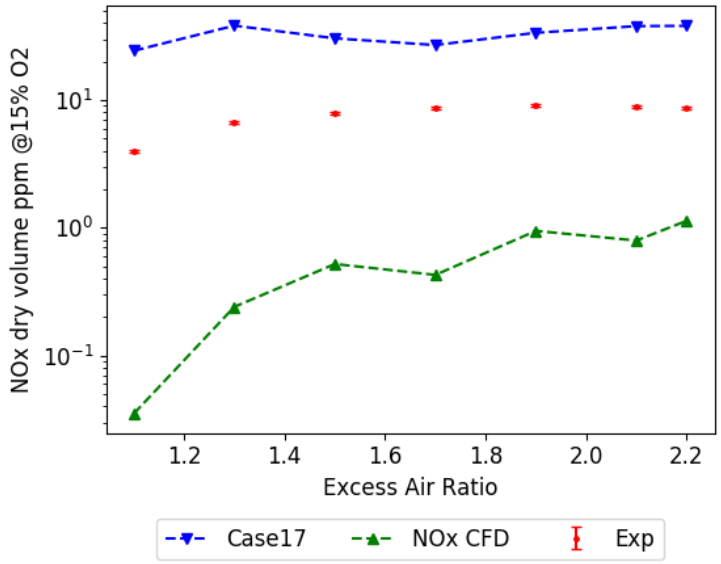
Detailed Chemical Mechanism: GRI-Mech 3.0
53 species, 325 reactions

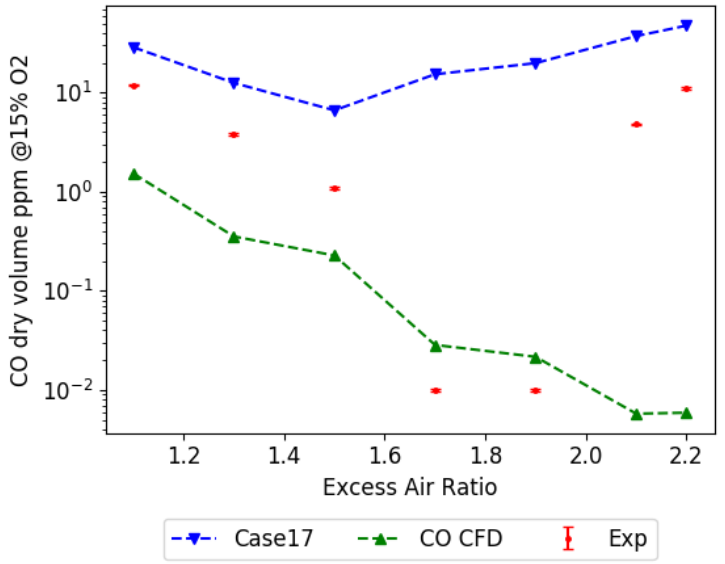


CRN

# *Comparison to CFD*

- CFD: FGM+NOx post processing
- CRN: GRI Mech 3.0

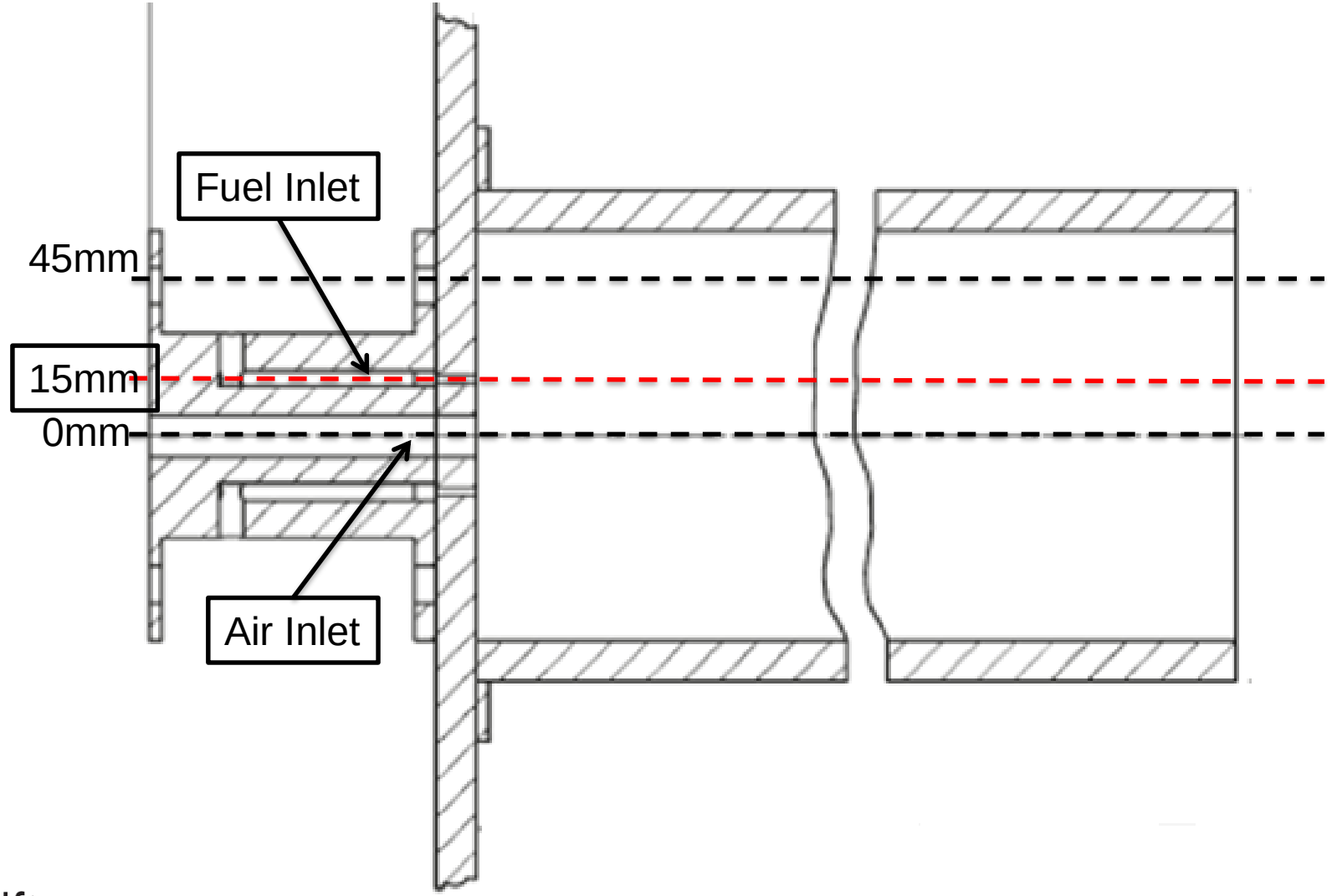


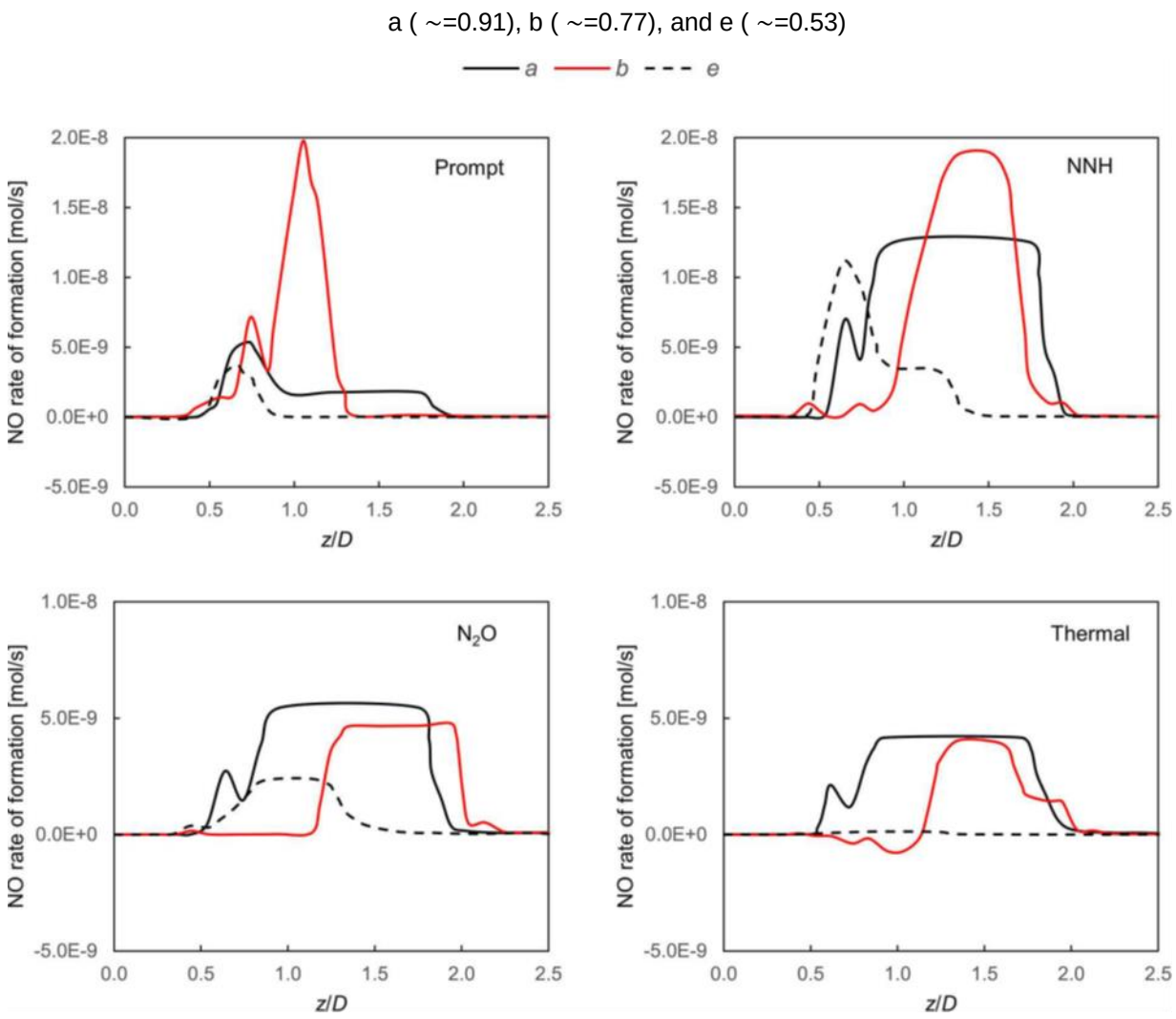
# NOx formation mechanisms

- Thermal pathway
  - $N_2 + O \rightleftharpoons NO + N$
- Prompt pathway
  - $CH + N_2 \rightleftharpoons HCN + N$
- NNH pathway
  - $N_2 + H \rightleftharpoons NNH$
- Reburn pathway
  - $CH + NO \rightleftharpoons HCN + O$

# Location in Combustor



# NOx pathways




- NOx formed in a section along the length of the combustor.
- Prompt and NNH pathways have a large contribution.
- Possible due to large number of reactors distributed in the domain based on physical phenomenon captured in CFD

[6] A AV Perpignan, R Sampat, A Gangoli Rao, Modelling pollutant emissions of Flameless Combustion with a joint CFD and Chemical Reactor Network approach, Frontiers in Mechanical Engineering 5, 63 November 2019, https://doi.org/10.3389/fmech.2019.00063

# Conclusion

- AGNES: Tool for CFD-CRN developed
- Application on a Combustor
- NOx and CO predictions closer to experiments than that from CFD
- Implementation of detailed Chemical Kinetic Mechanism enabled NOx formation pathway analysis which shows
  - location of formation
  - predominance of Prompt and NNH pathways.

***Thank You***