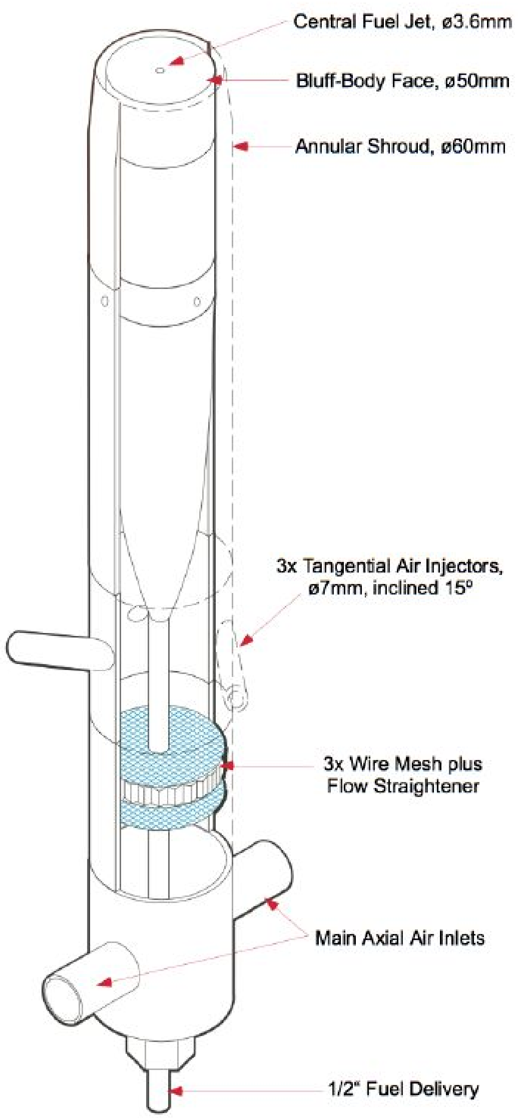
Numerical Simulation of Swirling Turbulent Combustion using Open Source Software

Richard Lozowy, Ph.D, E.I.T.
Fluids and Acoustics Analyst

1st Alberta CFD Users Meeting,
Edmonton, June 3, 2019

© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

Introduction

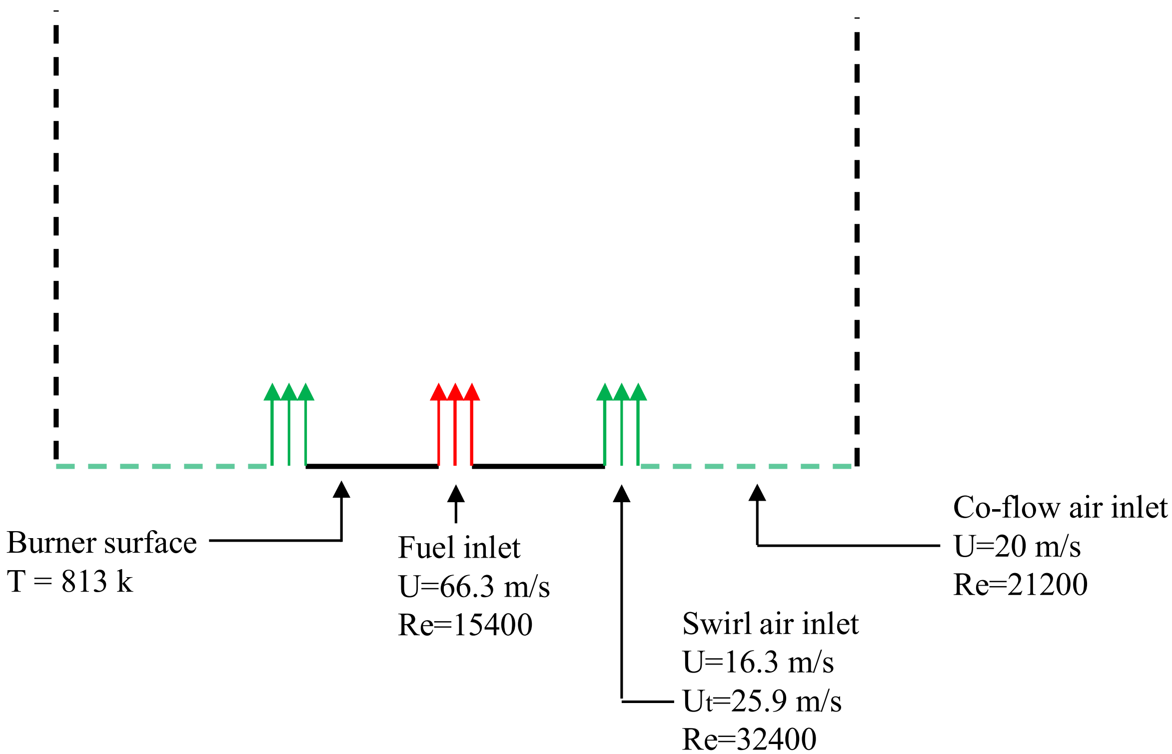


- Numerical simulation of a swirling diffusion flame is performed using open source computational fluid dynamics (CFD) software OpenFOAM.
  - This case is well documented and experimental data is available online (Masri et. al. 2004).
  - Good case for validation since it covers both combustion and complex turbulence in the swirling flow.
- The objective of this study is to gain a better understanding of turbulent combustion.
  - And also to verify that OpenFOAM can provide reliable results for combustion simulations.
- This presentation is a continuation of the work done in a M.Sc. Thesis (Paladin 2012) that was completed for GDTech Engineering (Belgium).

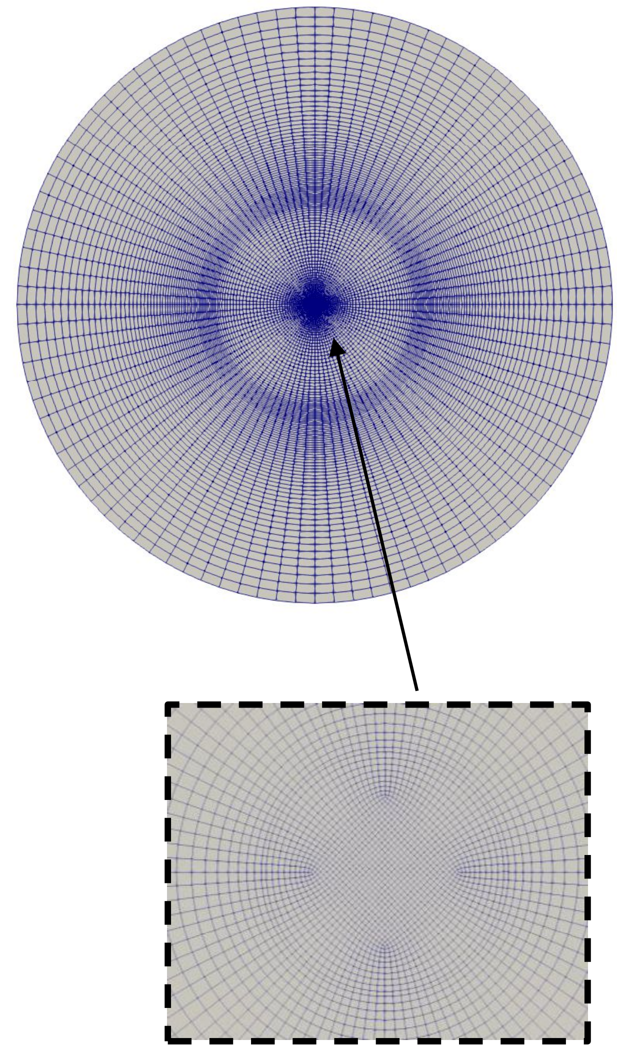
© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

Model description

- Fuel is methane.
- Large-eddy simulations (LES) using WALE model.
- Unsteady RANS (URANS) using k-e model.
- Uniform velocity conditions used at inlets.



Cross-section of hexahedral grid



Grid at inlet

Limitations of using OpenFOAM for Combustion

- OpenFOAM combustion has a majority of the functionality found in commercial codes.

- However, the current release of OpenFOAM does not steady state solver for combustion.

- For transient simulation CFL number < 1.

$$CFL = \frac{U\Delta t}{\Delta x}$$

- This means that combustion simulations with OpenFOAM will typically be longer, i.e. 10000s of timestep to develop the flow.

- OpenFOAM can also run transient simulations with large timesteps (CFL>>1).
  - Stable large timestep simulations can be run without specifying the timestep.

© AP Dynamics Inc. – April 2019 – www.ap-dynamics,net

- Single step irreversible reaction mechanism.

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

- GRI mechanism consists of 53 species and 325 reversible reactions.
  - Includes details on NOX.

- Bilger's mechanism consists of 15 irreversible and 10 reactions.
  - Does not calculate NOX.

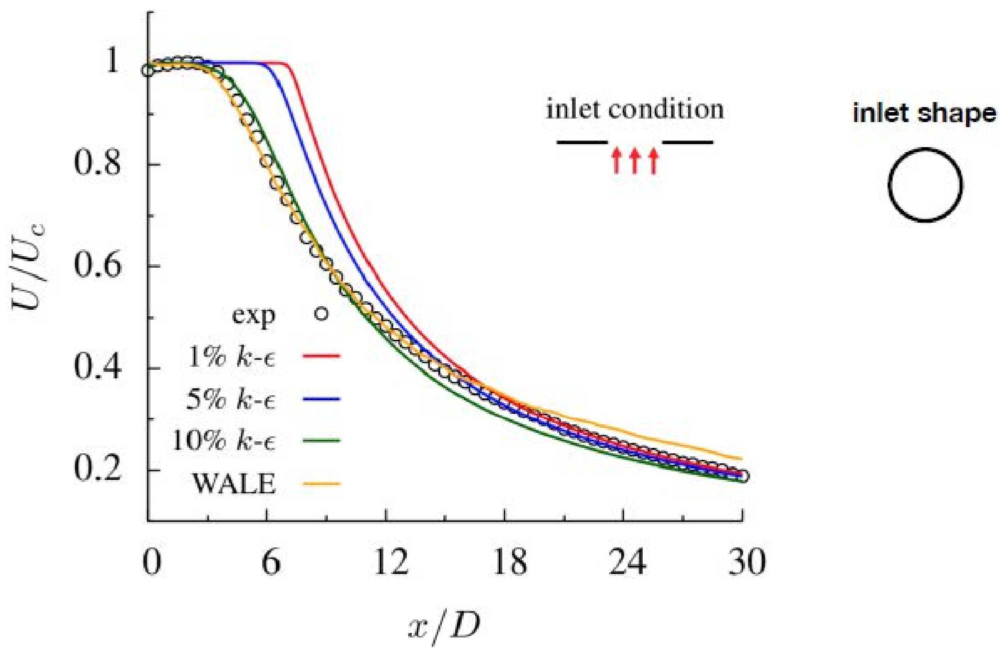
- A model is required to represent the turbulent-chemistry interactions at the micro-scale.
  - Two common combustion models are tested here: the Eddy Dissipation Concept (EDC) and the Partially Stirred Reaction (PaSR) model.

Literature review of isothermal low-Reynolds number jets

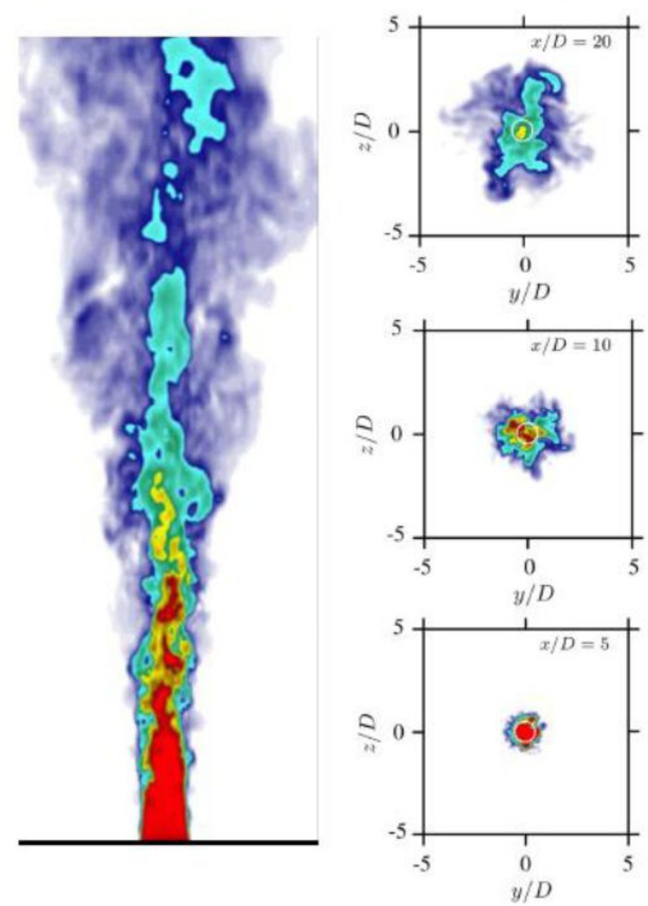
- LES compares well with experimental data.
- RANS also compares well when a high turbulent intensity is imposed at the inlet.
  - Low turbulence at the inlet increases the length of the laminar region.

From CFD Canada conference 2018, Lozowy et. al.

Experimental data provided by Dr Tachie at University of Manitoba



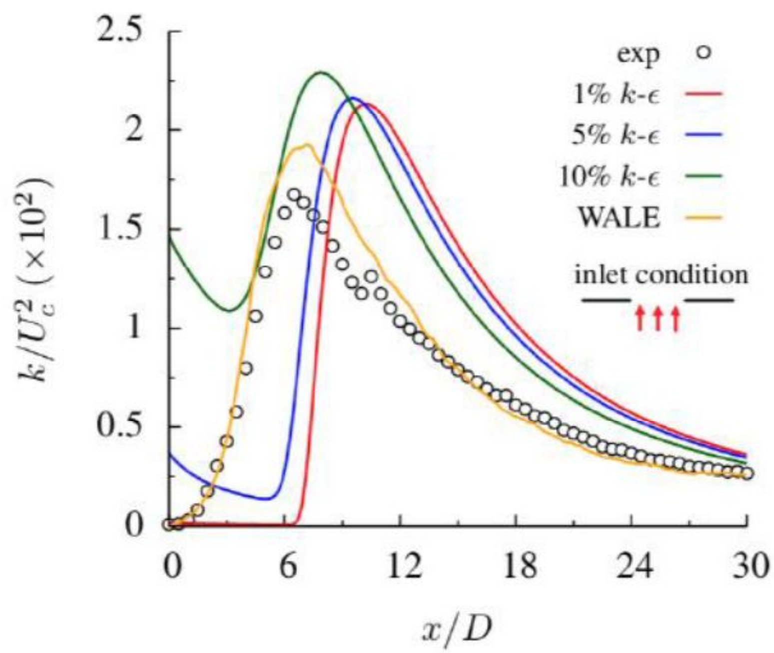
snapshot of instantaneous velocity from LES



© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

Literature review of isothermal low-Reynolds number jets

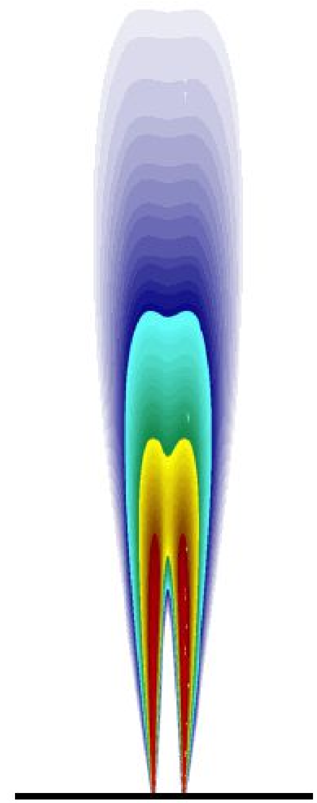
- LES captures the laminar-to-turbulent transition at the inlet.
  - Even though no turbulence is imposed at the inlet.
- RANS does not capture the transition.
  - However TKE profile is comparable.



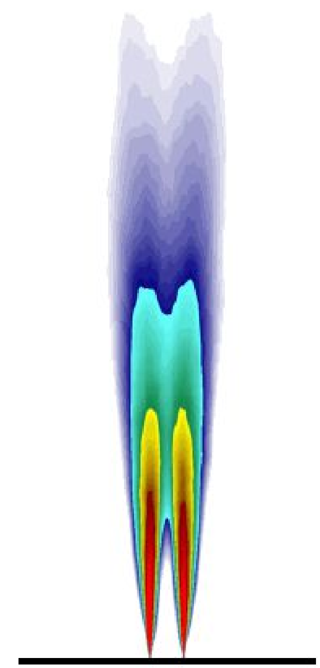
From CFD Canada conference 2018, Lozowy et. al.

Experimental data provided by Dr Tachie
at University of Manitoba

TKE from RANS k-ε model (5% inlet turbulence)



TKE from LES WALE model (laminar inlet)



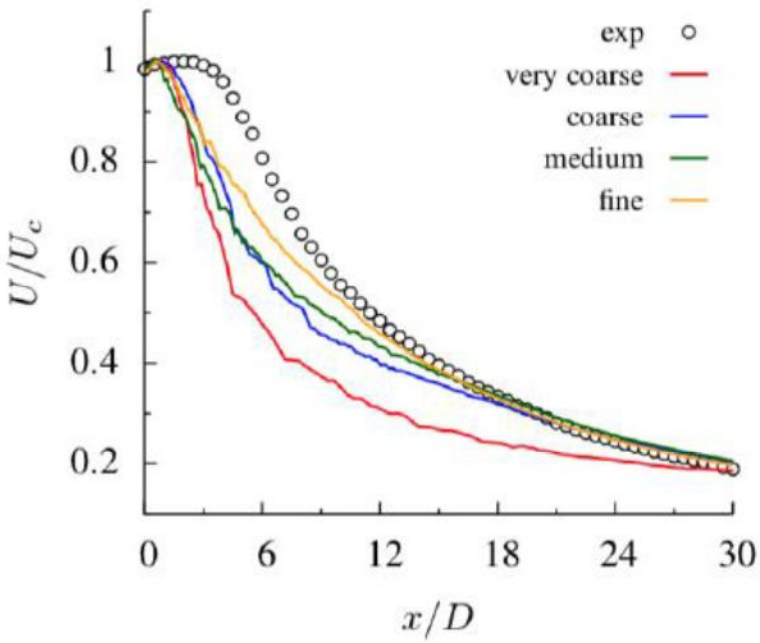
© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

Literature review of isothermal low-Reynolds number jets

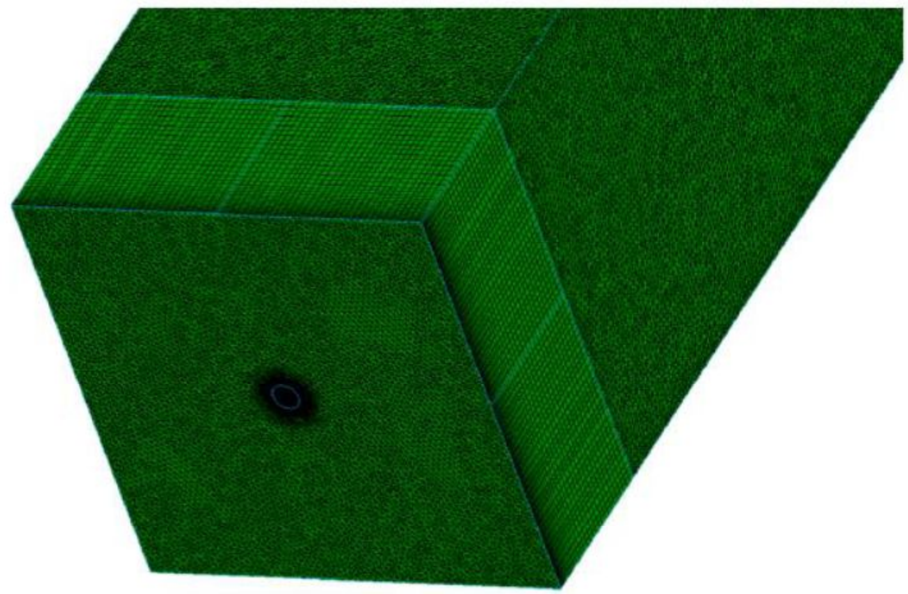
- Getting good results with RANS is still dependent on using a high-quality grid.

From CFD Canada conference 2018, Lozowy et. al.

Centreline velocity from grid independence study using tetrahedral cells only.

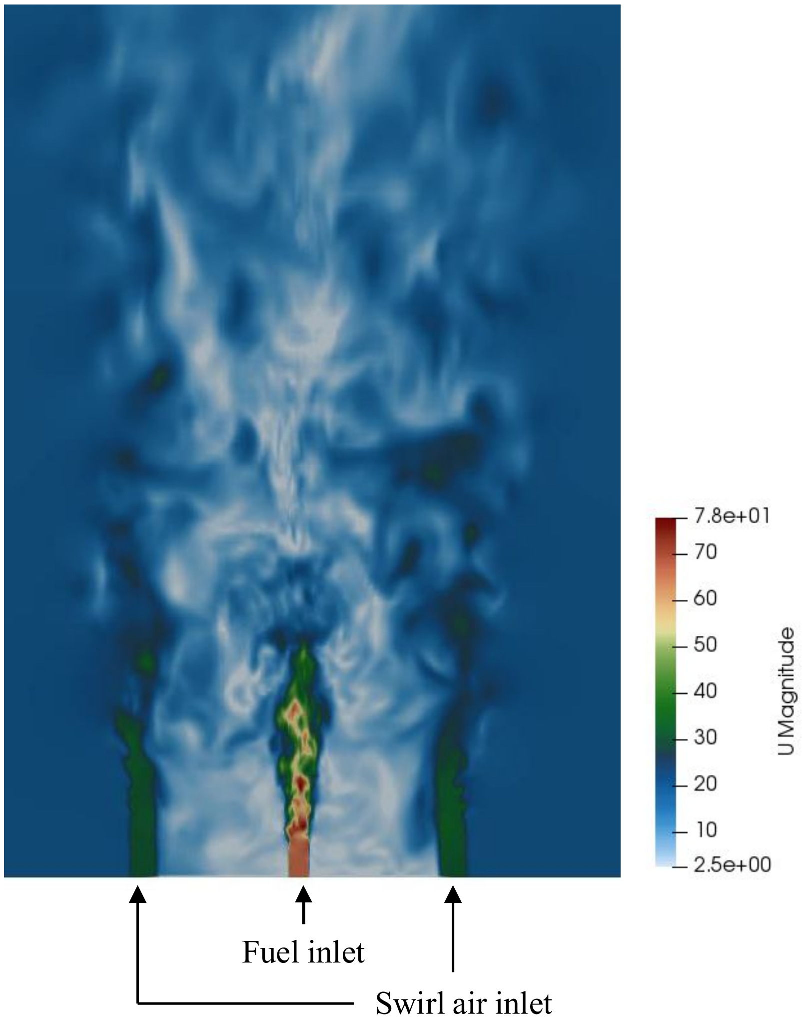


A thick layer of prism cells fixes this issue.

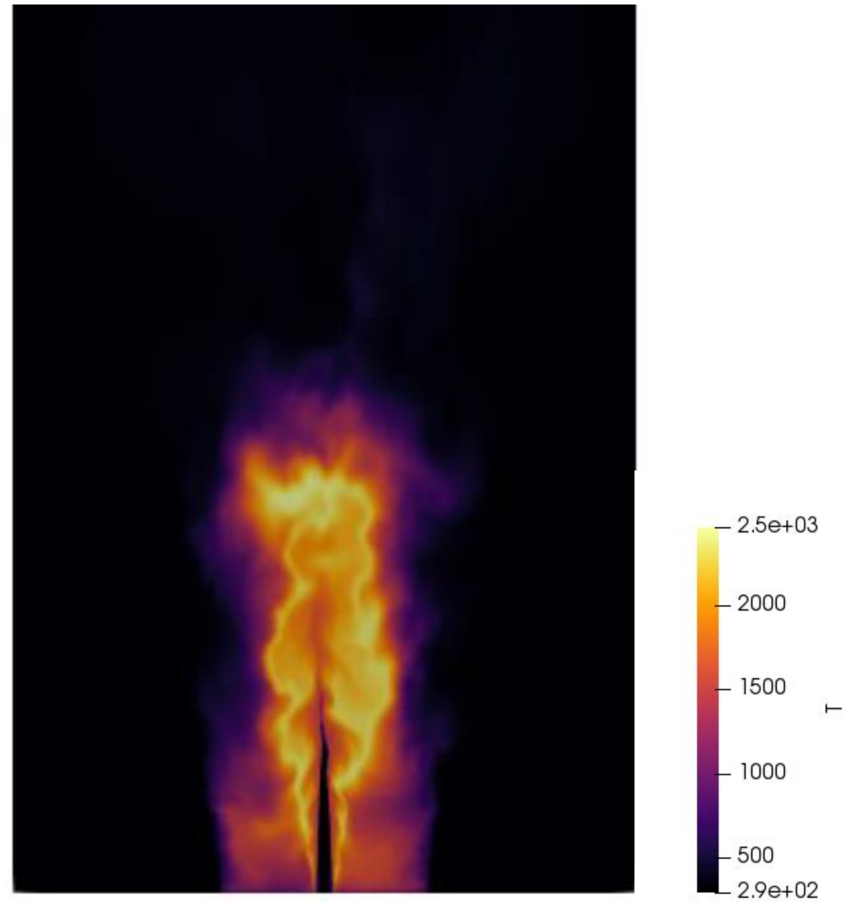


Instantaneous LES results

velocity field

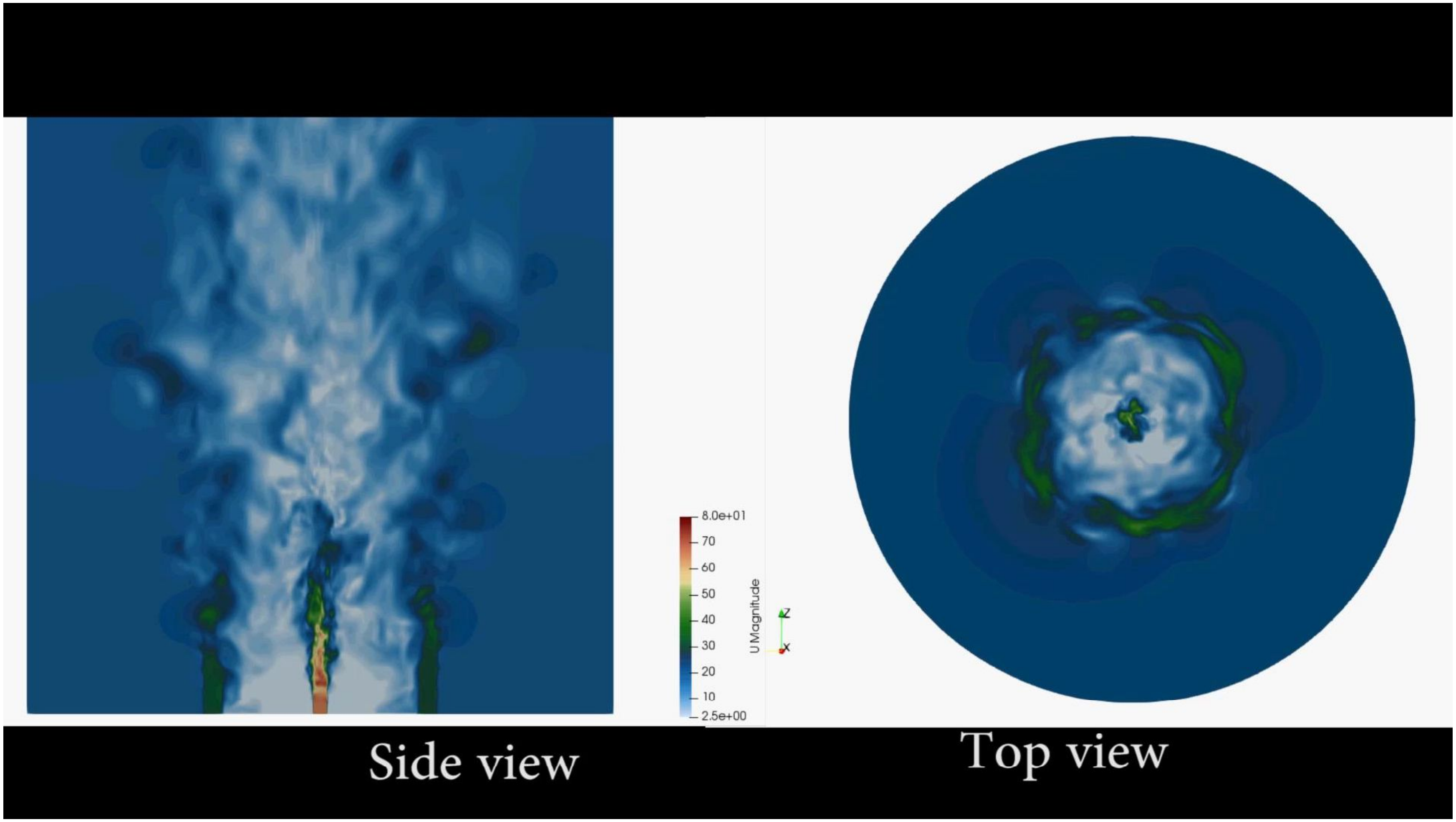


turbulent flame (single step reaction)



© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

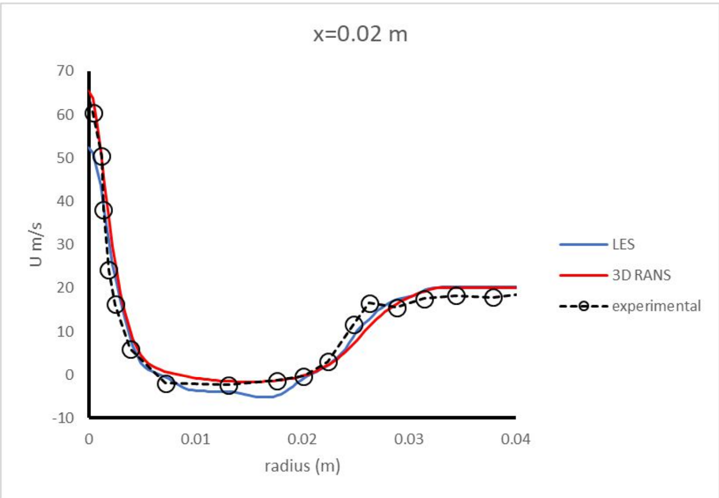
Instantaneous LES results

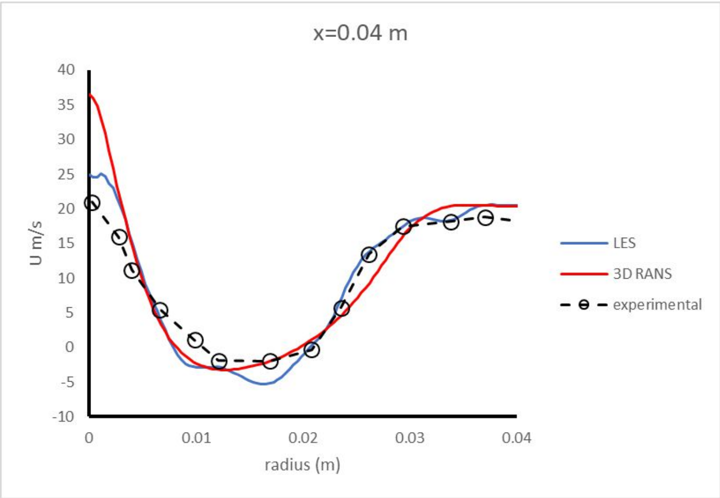


© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

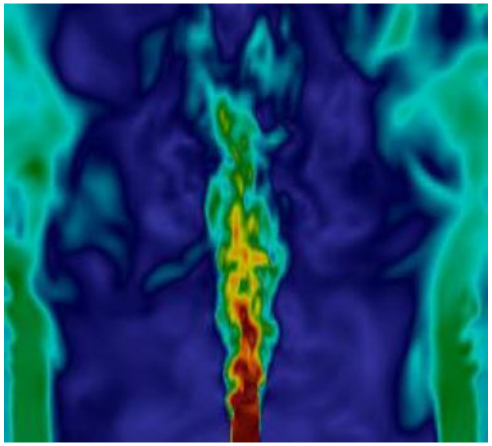
Velocity profiles from 3-D isothermal case

- Overall both LES and URANS provide a reasonable prediction of the velocity prior to the ignition of the flame.

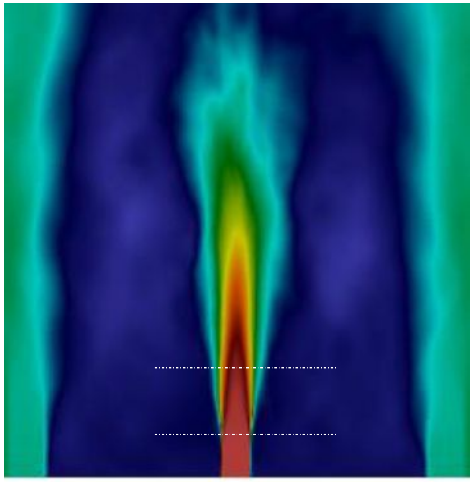




Instantaneous LES velocity



Time-averaged LES velocity



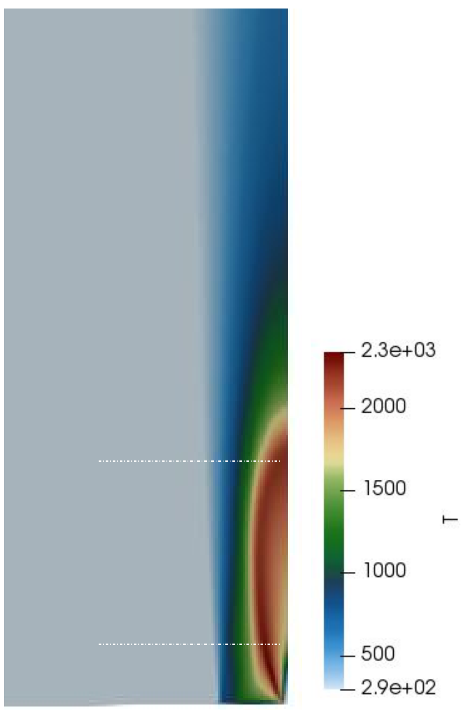
- The RANS does not capture the decay in the centreline velocity.
  - But that was also expected considering the limitations of RANS.
- When the flame is ignited, this affects the velocity profile by increasing the length of the jet.

© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

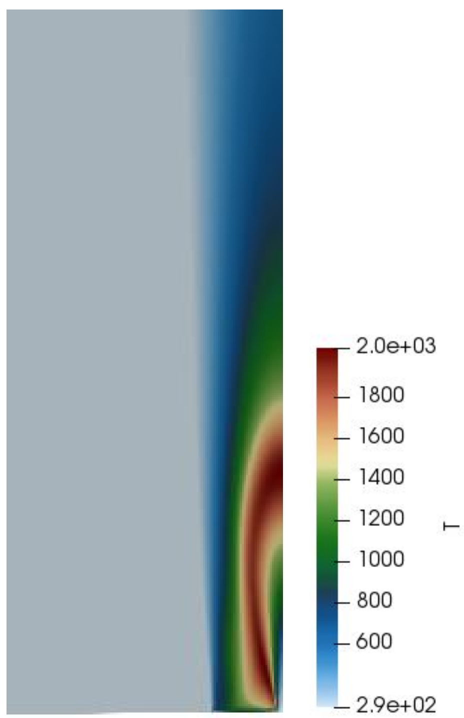
URANS temperature contours

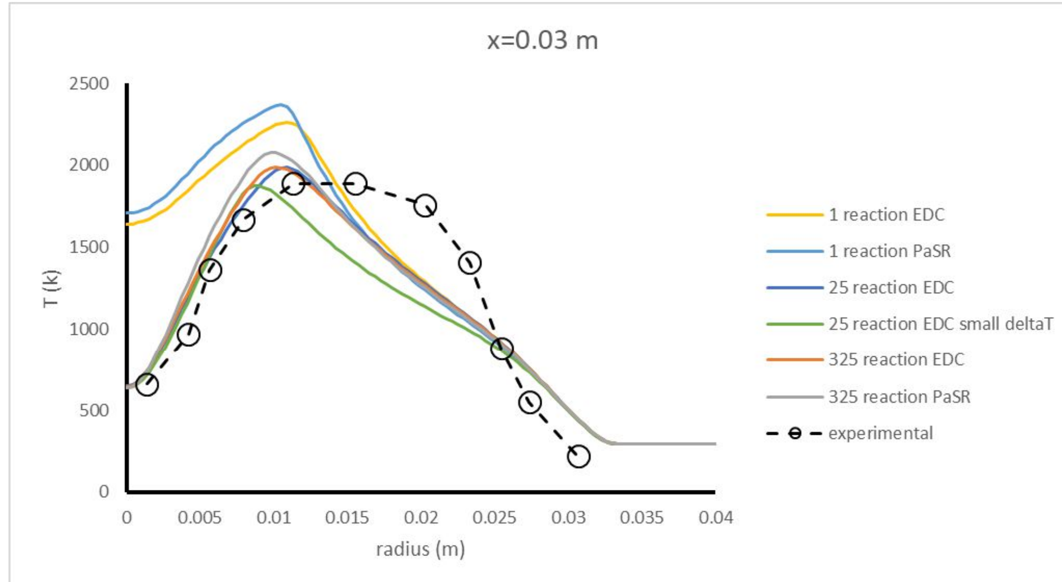
- The single step reaction mechanism does not fully capture the shape of the flame.
  - Temperature is over predicted, relative to experiments.

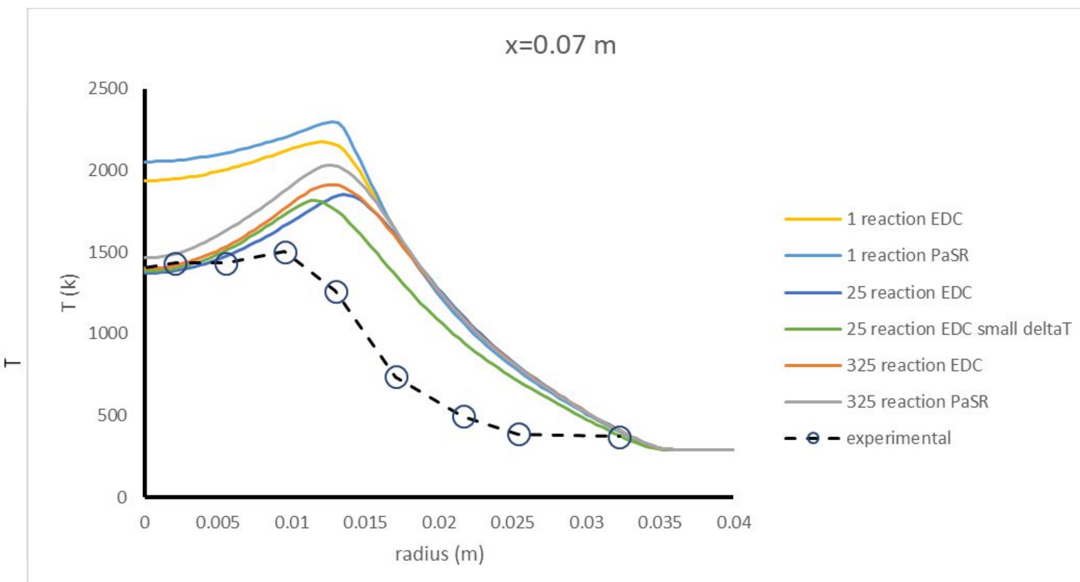
Single step reaction mechanism (2D case)



GRI 325 reaction mechanism (2D case)





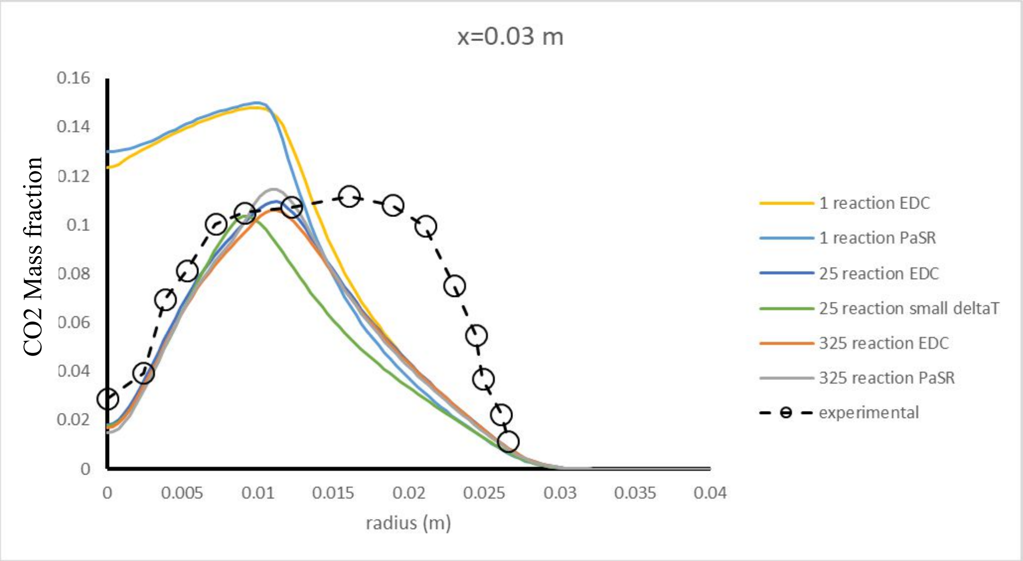


© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

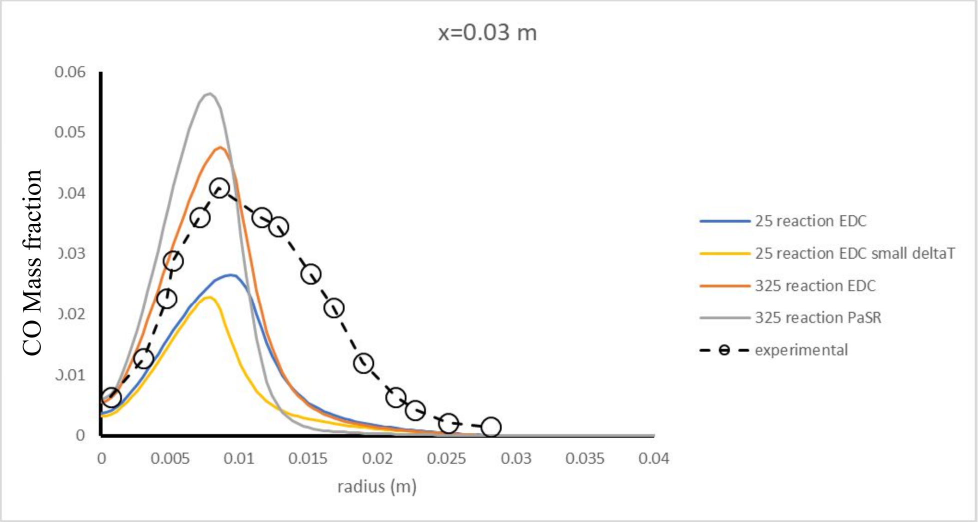
Combustion products

- CO2 is reasonably calculated when using 25 and 325 reactions.
- It appears that to obtain accurate results for the minor species, more reacting mechanisms are required.
  - However NO is overpredicted even when using 325 mechanisms.

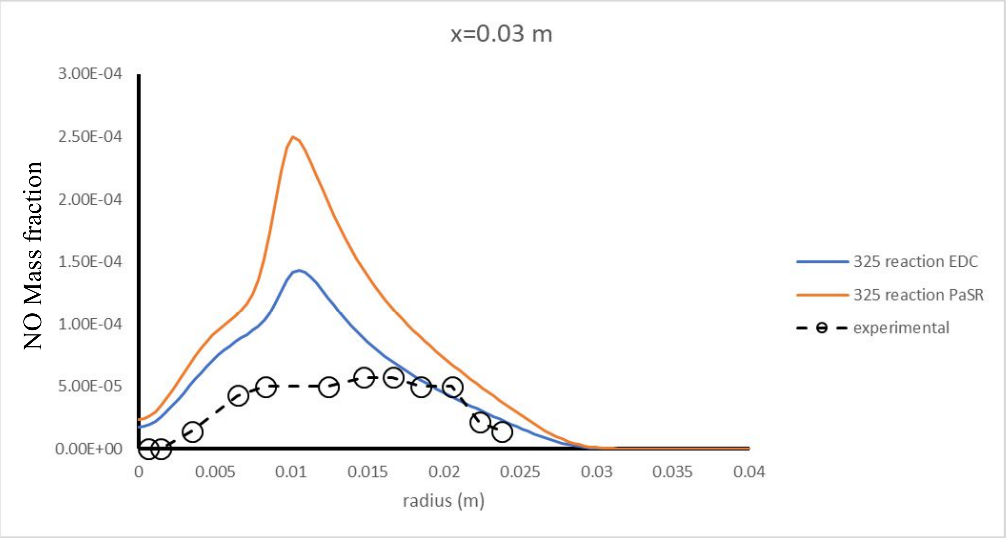
CO2



CO



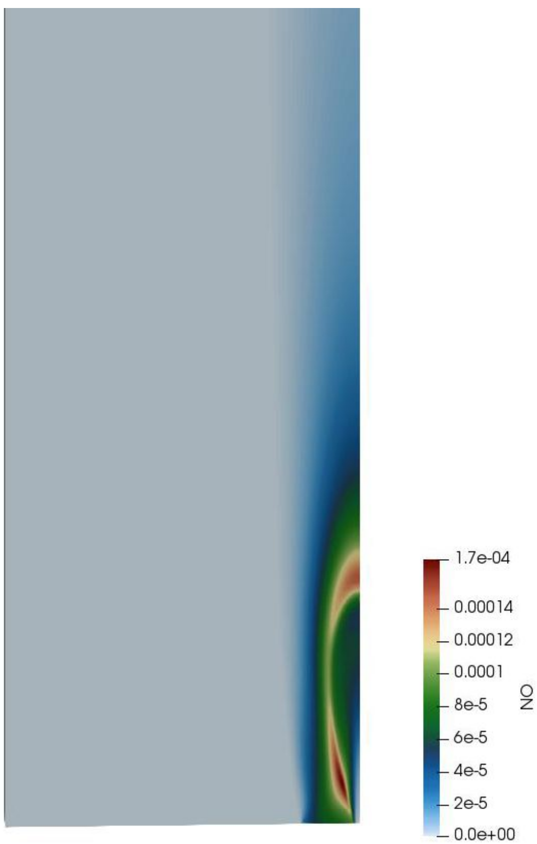
NO



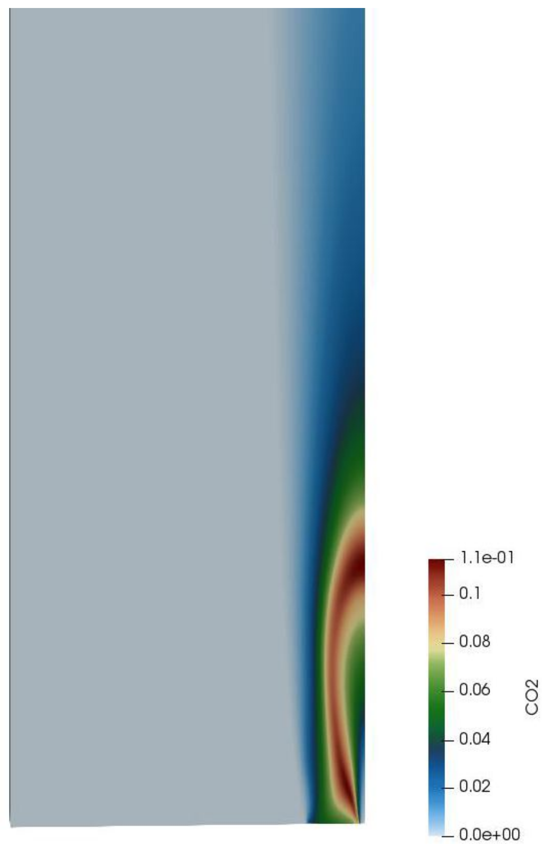
© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net

Combustion products

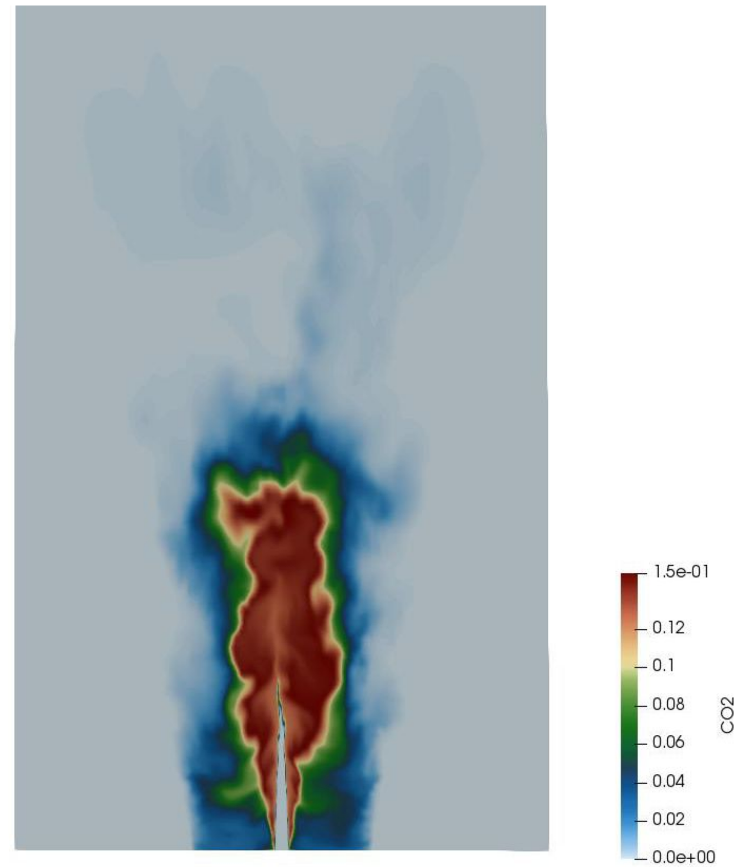
RANS GRI 325
NO contour



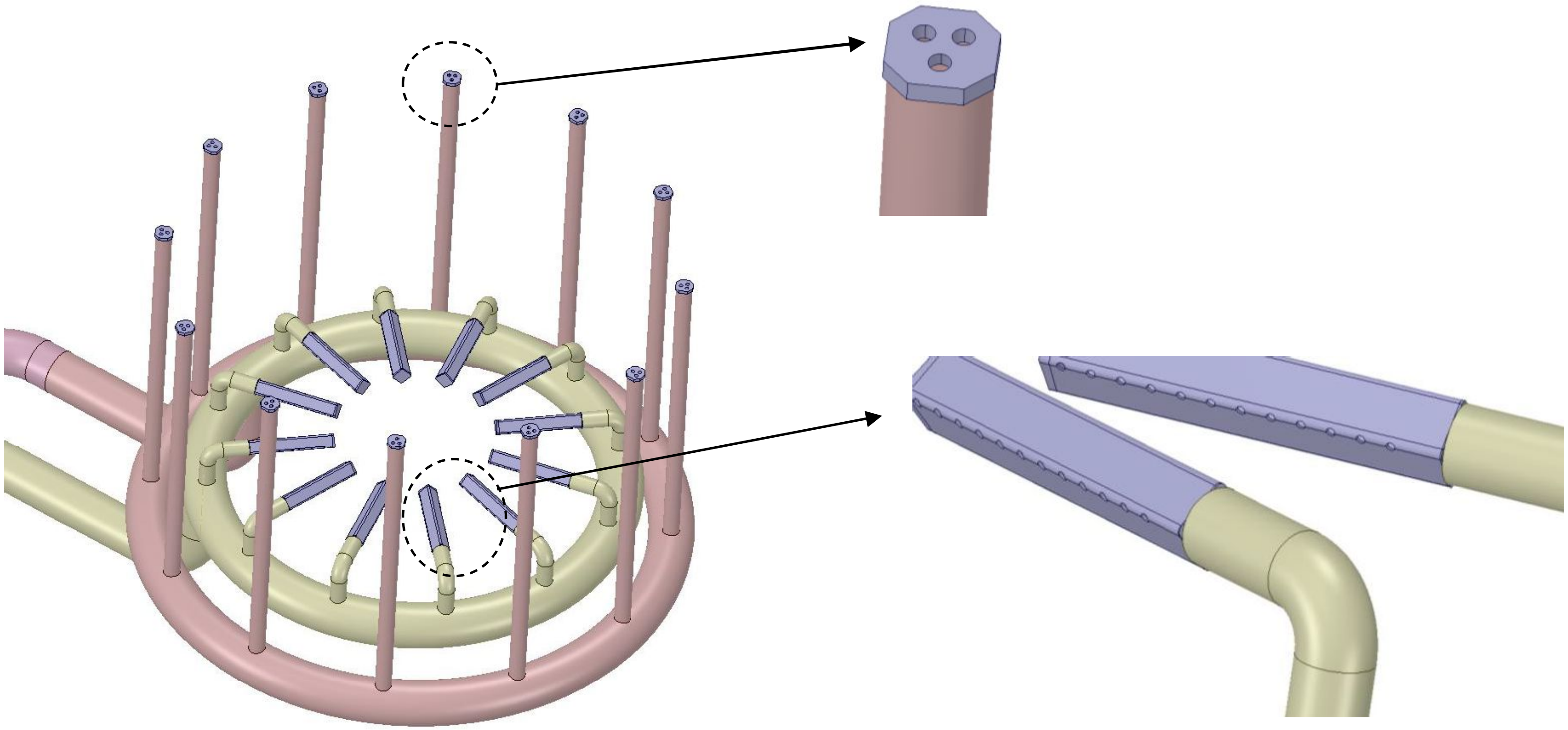
RANS GRI 325
CO2 contour



LES single step
CO2 contour



Industry applications



- Significant number of nozzles on Industrial burners.
  - For the above example there are 324.

- The complexity of the combustion model needs to be weighted against what is feasible for large domains.

© AP Dynamics Inc. – April 2019 – www.ap-dynamics,net

Conclusion

- OpenFOAM is capable of providing reliable results for combustion simulations.
  - The single step mechanism gave a substantially higher temperature and is therefore not suitable.
  - The GRI 325 mechanism is too computationally intensive.
  - The Bilger's 25 mechanism appears to be a good compromise in complexity.

- Running OpenFOAM simulations with large timesteps overcomes the lack of a steady state combustion solver.

Future steps

- Further works needs to be done on the LES.
- Mechanism with 5 reactions will be compared to Bilger's 25 mechanism.
- Equations to calculate NOX indirectly will be implemented.
  - GRI mechanism is not required to obtain NOX.

© AP Dynamics Inc. – April 2019 – www.ap-dynamics.net