Update since workshop

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Nov 15th, 2011

N-heptane spray modelling with Lagrangian probability density function approach

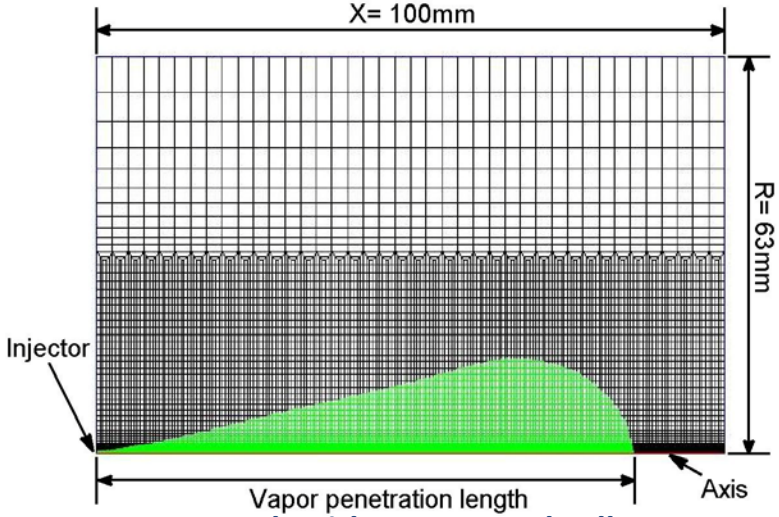
➢ The reasons for choosing TPDF approach:

- Naturally accounts for turbulent fluctuations
- Resolves the problem of closure of the chemical source
- Good performance has been demonstrated in simpler but related flames in the TNF workshop - “Cabra burner” flame (H_2 and CH_4)

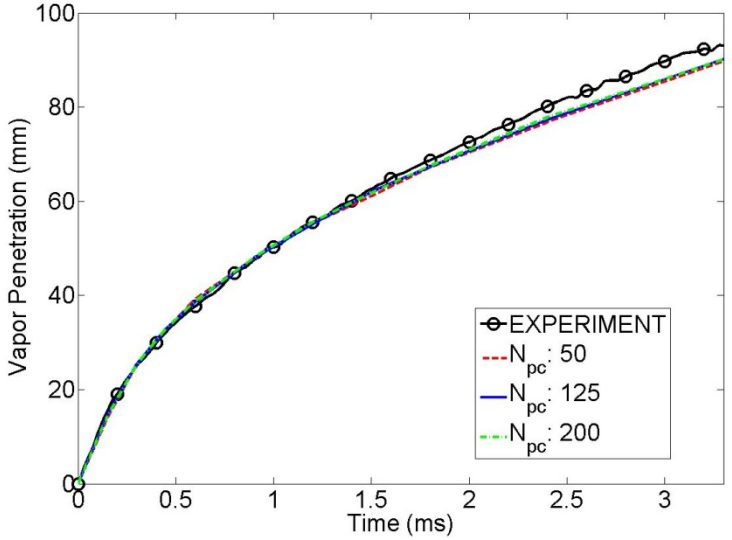
➢ Implementation

- Fluent v13.0 commercial code
- Gas jet method (Abraham and Pickett, 2010)

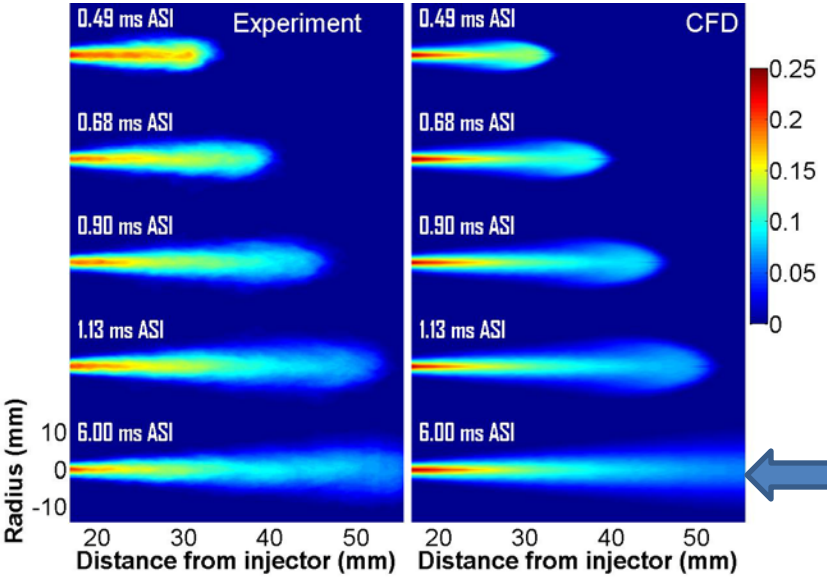
Mesh: 2D axisymmetric



Mesh with 10320 total cells



Vapor penetration length prediction



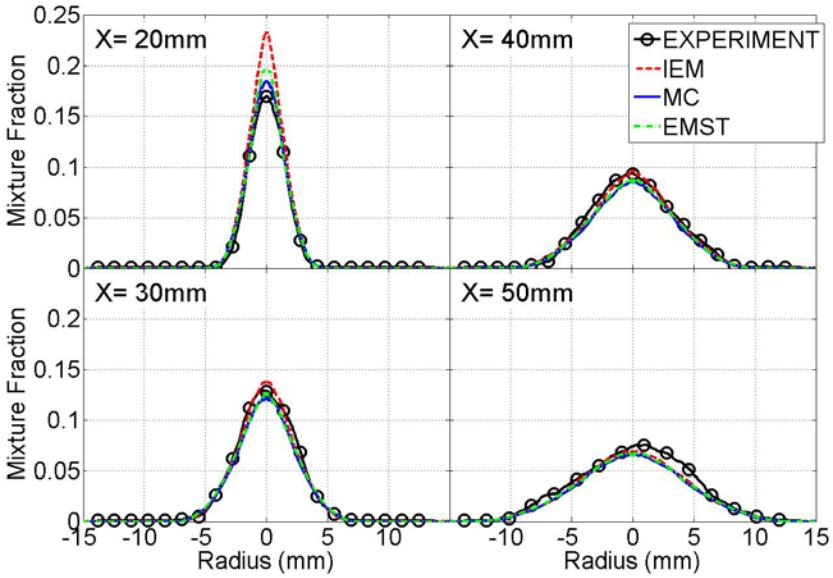
Fields of fuel mixture fraction from experiments and computations with the EMST mixing model on mesh 2, Cø=2.5

Vapor penetration length:

- ECN definition (0.1% of fuel mass fraction)
- Can capture the transient process within first 0.2ms
- Slightly under-predicts after 2ms

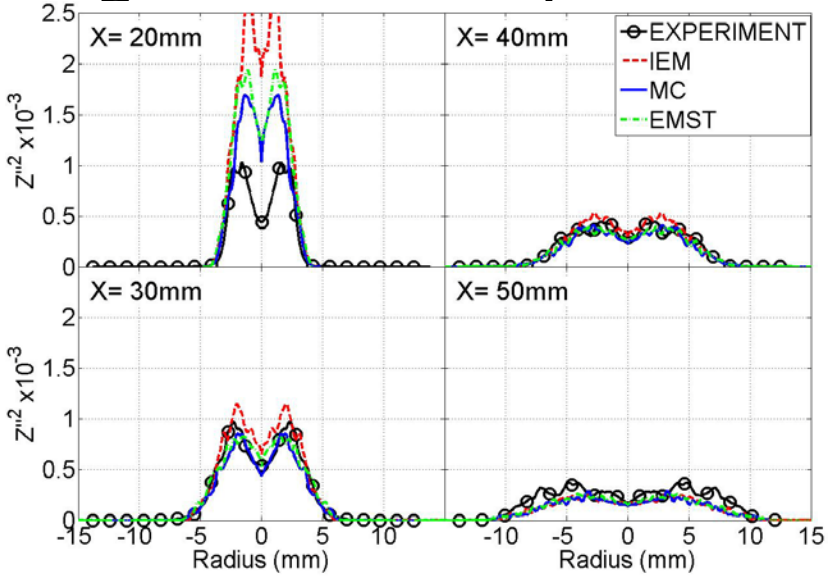
Qualitatively captures the experiment on the spatial and temporal structures

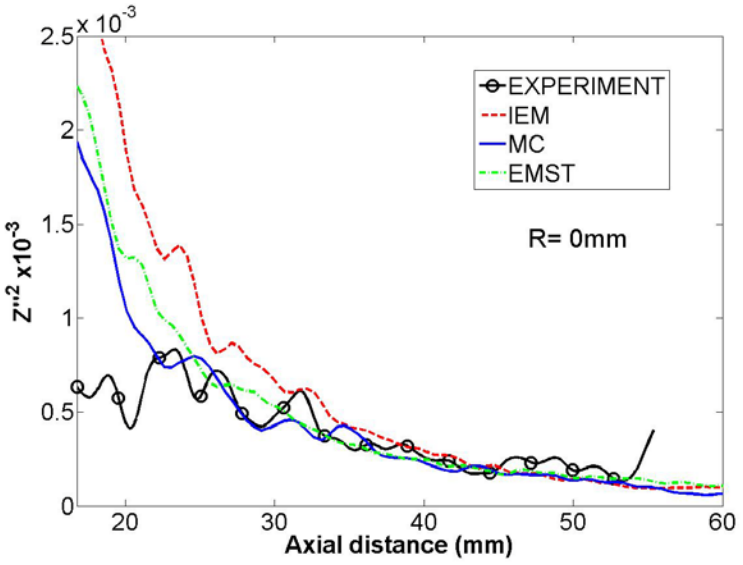
Non-reacting case: mixing models study



Radial profile of fuel mixture fraction from experiments and computations with different mixing models at Cϕ=2.5

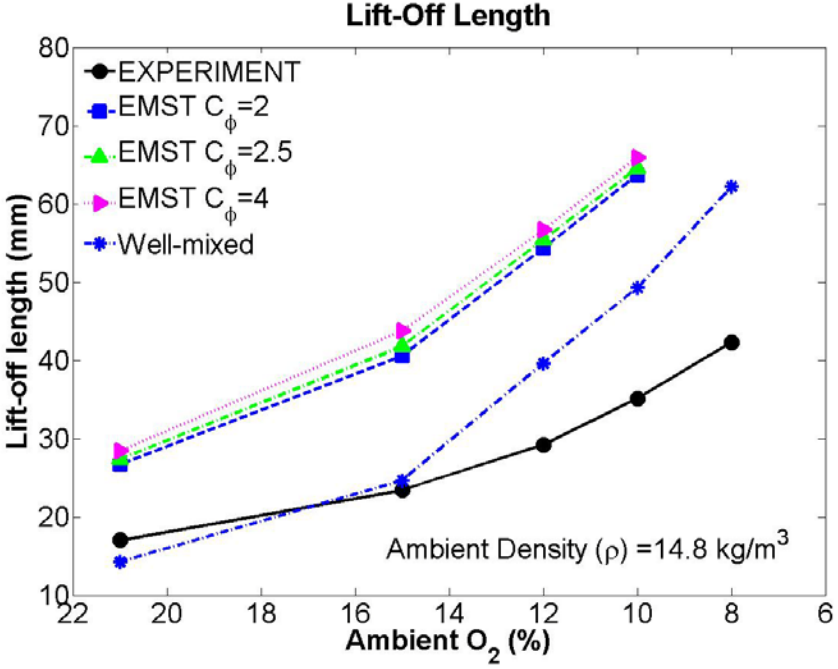
The three different mixing models can capture the experimental variance very well except that the IEM mixing model over-predicts the result before around 30mm

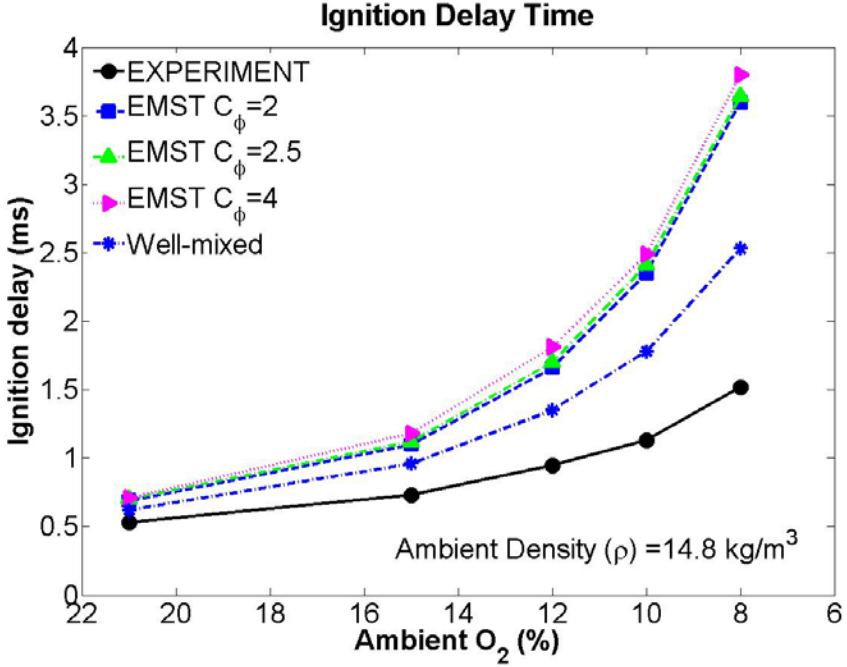




Radial and axial profile (R = 0mm) of fuel mixture fraction variance from experiments and computations with different mixing models at Cϕ=2.5

ERC29-mixing constant study-EMST

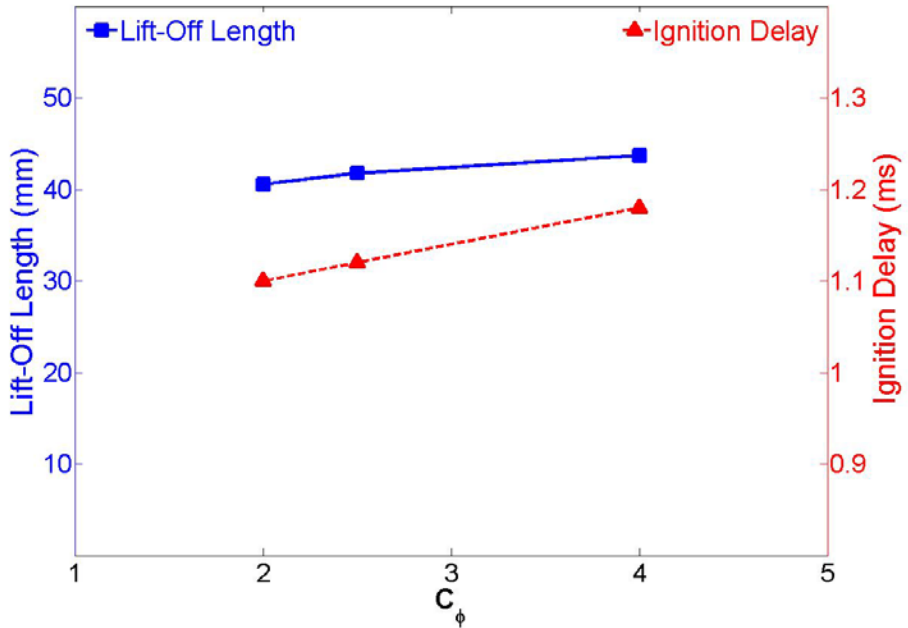




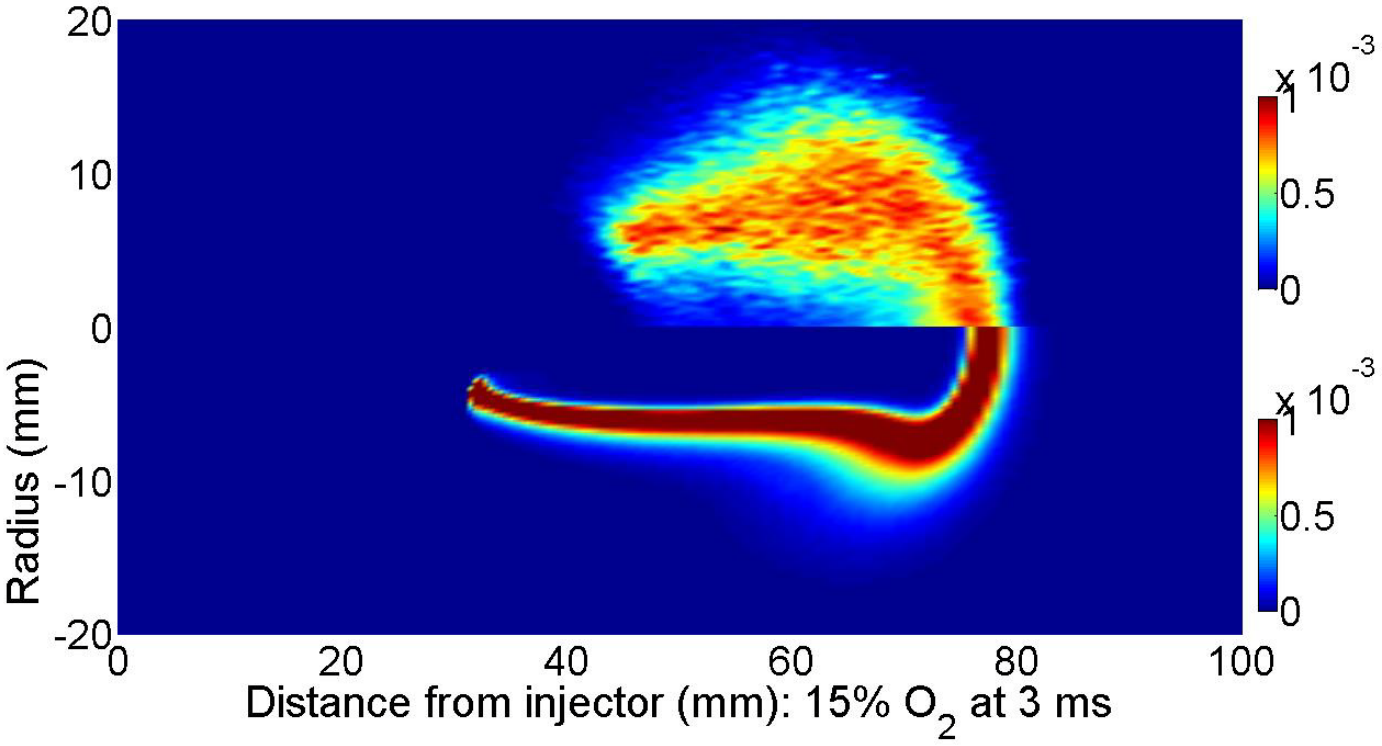
- There is a big difference between well-mixed and the PDF method.

- Preliminary results with the pdf method are not actually better than a well-mixed model.
- However, we need to investigate a more detailed chemical model.

- Effect of mixing rate (C_ϕ):
  - Ignition was postponed with bigger C_ϕ
  - LOL become longer with bigger C_ϕ



OH contour comparison-ERC29

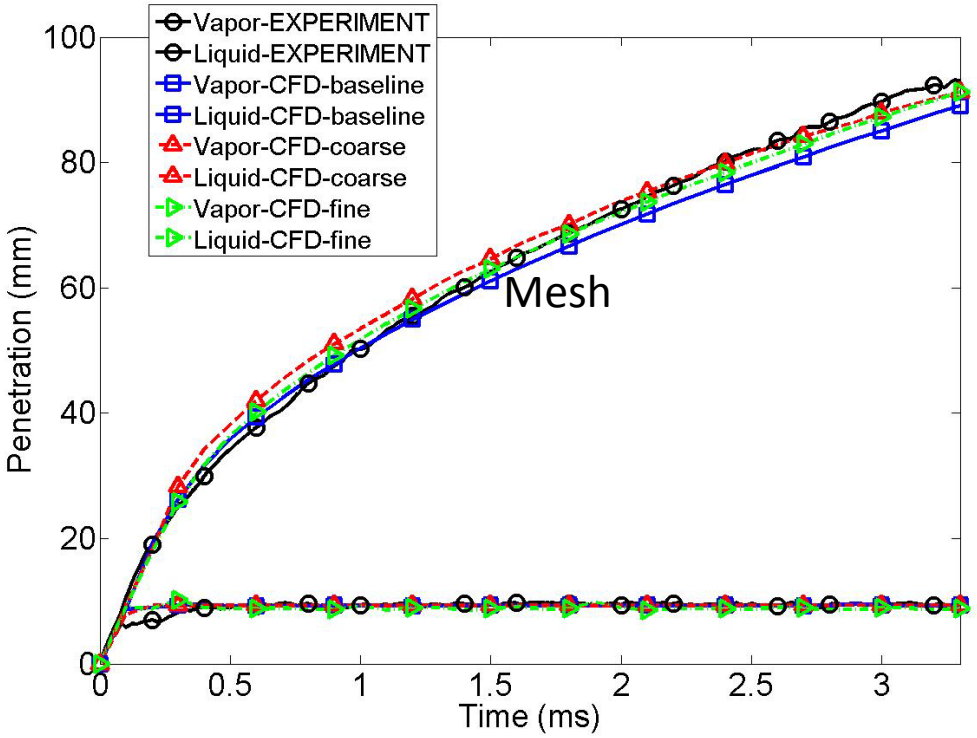


Upper plot is PDF and lower one is well-mixed model.

- There are larger, qualitative structural differences.
- PDF method appears more correct, intuitively.
- Can experiments expose these differences?

Progress in implementing ECN definitions

Penetration for LPEF method



- ✓Well mixed model
- ✓ECN definition:
  - •Liquid length: 0.1% fuel mass fraction
  - •Vapor penetration length: 0.15% liquid volume fraction
- ✓Liquid length is independent of mesh
- ✓Liquid length is independent of definition chosen, e.g. also independent of mesh with other definitions, like the definition of “leading particle position” .

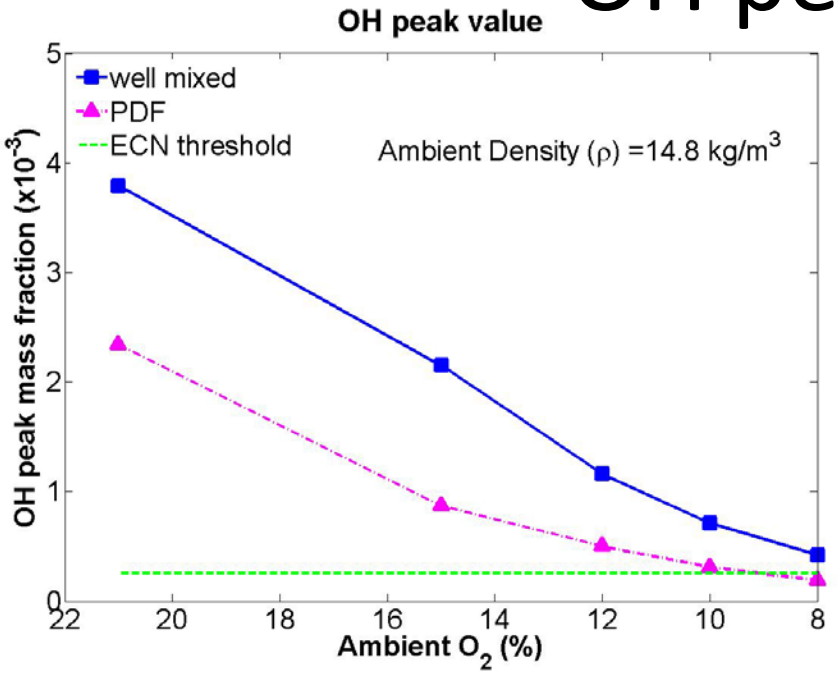
Mesh resolution:

Coarse: 6300

Baseline: 25200

Fine: 100800

OH peak value



With PDF method, at 8% O2, the maximum OH is below the threshold 0.00025.

0.0001 or less for OH threshold seems more appropriate for PDF method