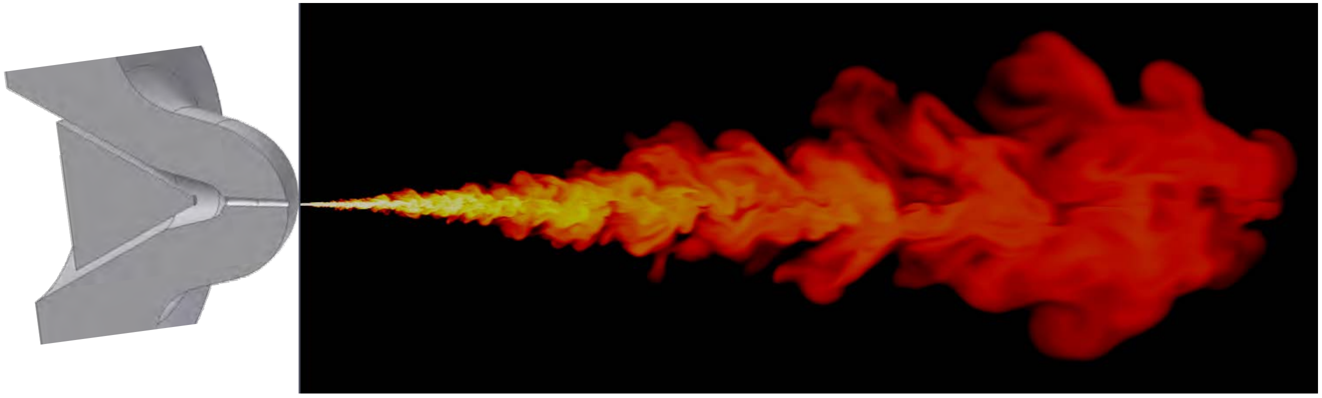
Advanced CFD Modelling of Diesel-like Reacting Sprays in OpenFOAM

Third Two-day Meeting on
Internal Combustion Engine Simulations Using OpenFOAM® Technology
February 22nd-23rd, 2018



UNIVERSITAT POLITÈCNICA DE VALÈNCIA

CMT motores térmicos

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R. Novella
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E. Pérez-Sánchez

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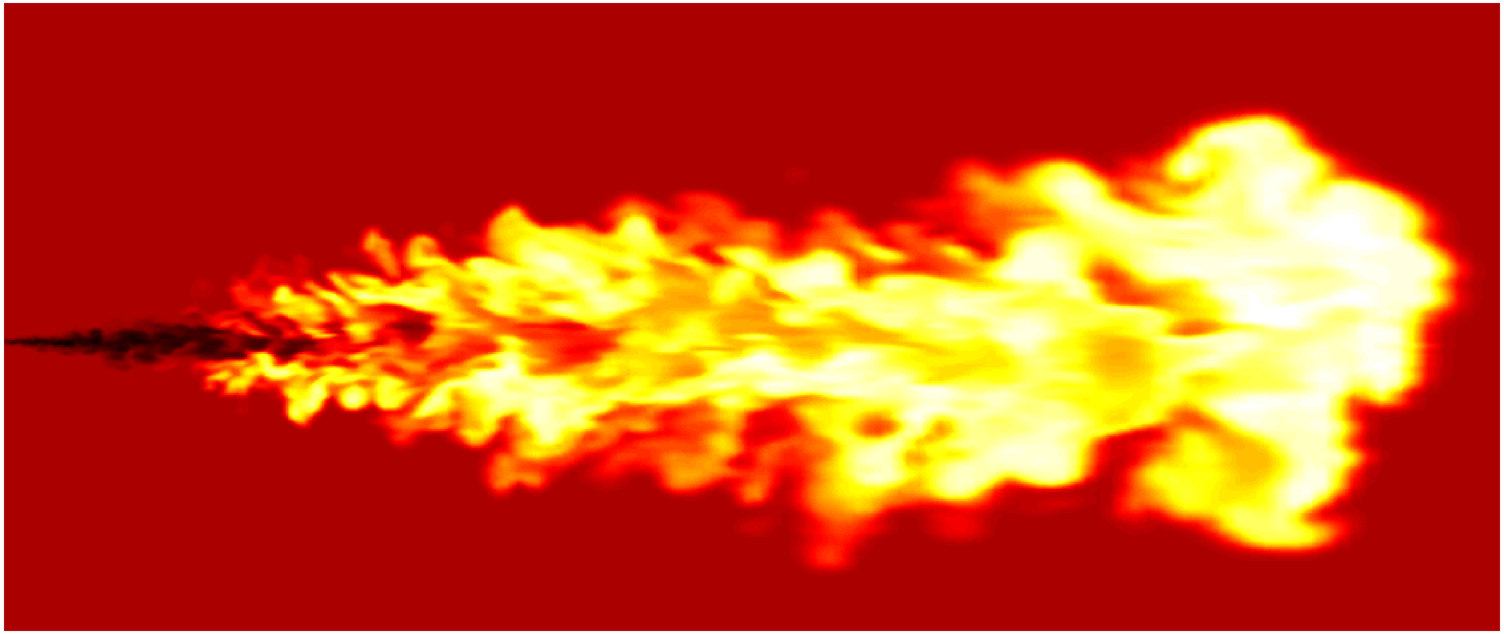
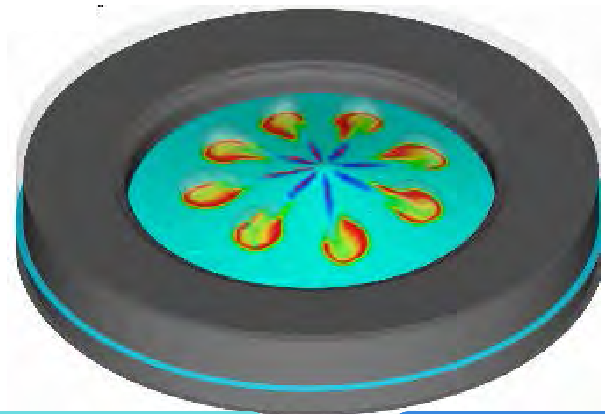
- Background and approach
- Spray Modelling
- Combustion Modelling



BACKGROUND

CFD of combustion in Diesel engines still a challenge:

- Complexity of the physical and chemical fundamental processes in a highly transient environment



INTERNAL FLOW
- Cavitation

MIXTURE FORMATION
- Liquid breakup
- Evaporation
- Momentum transfer

COMBUSTION
- Turbulent mixing
- Chemistry

POLLUTANT EMISSIONS

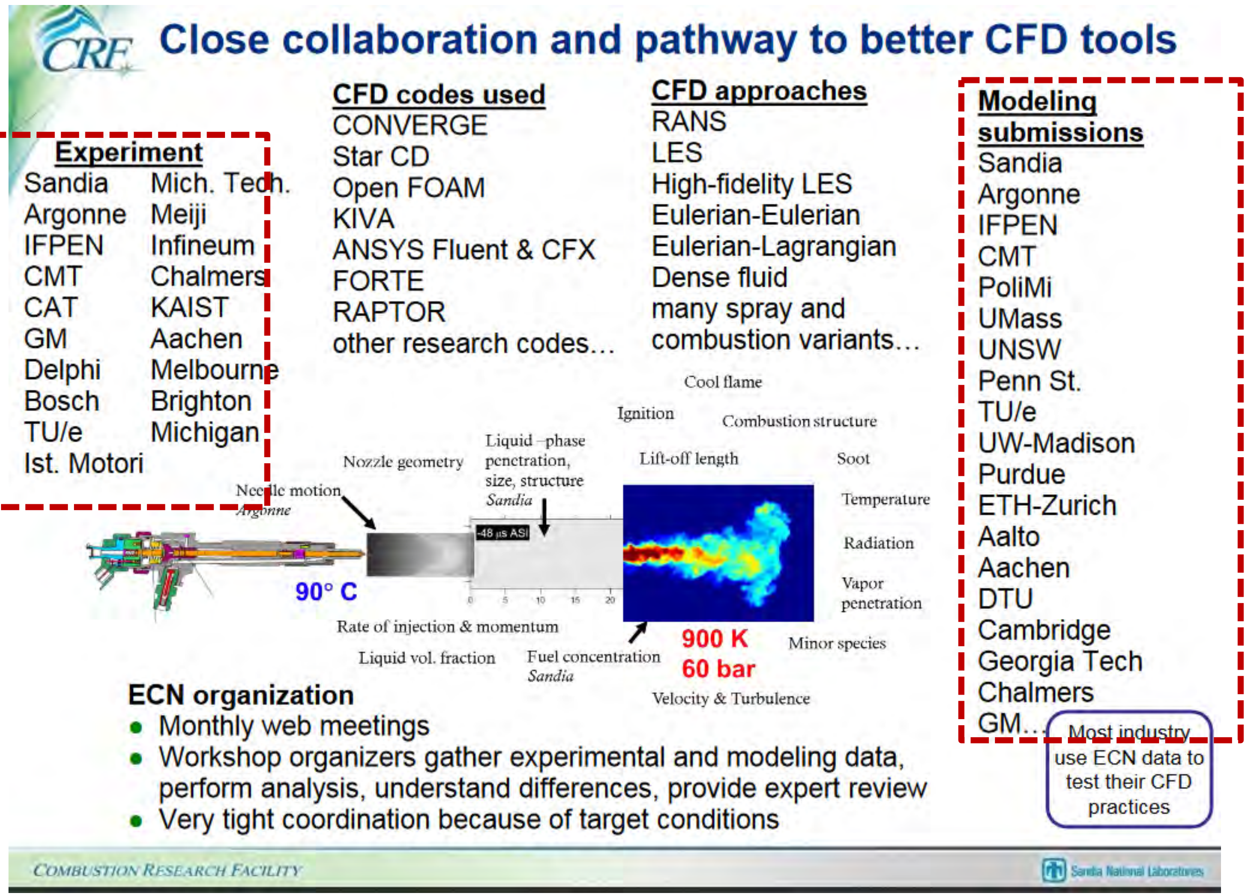
IN-CYLINDER BOUNDARY CONDITIONS:

Piston displacement, spray-spray & spray-wall interactions,…

Engine Combustion Network (ECN)

- Necessary dialogue between research efforts

Experiments | Calculations

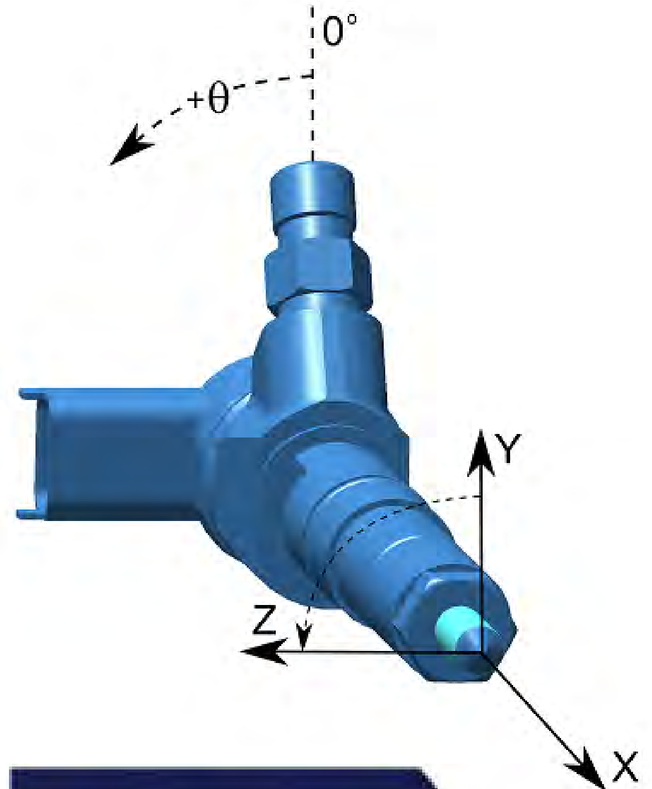


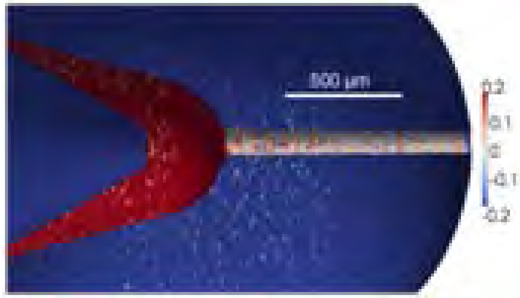
Engine Combustion Network (ECN)

- Spray A condition
  - Single-hole injector
  - Typical Diesel combustion conditions

Injection	Value
Nozzle diameter [μm]	90
Injection pressure [bar]	500-1500
Injection duration [ms]	1.5 / 5

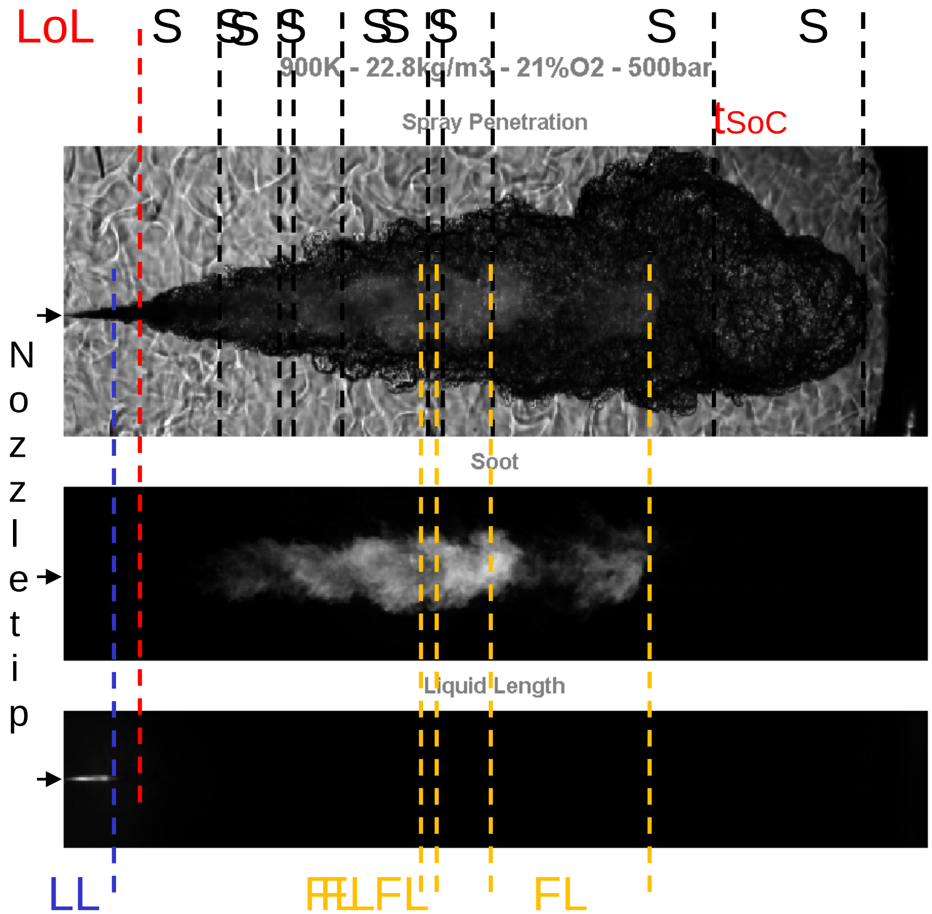
Ambient	Value
Pressure [bar]	60
Temperature [K]	700-1000
Density [kg/m³]	22.8
O_2 [%]	13-15-21





Diesel combustion, a highly transient process

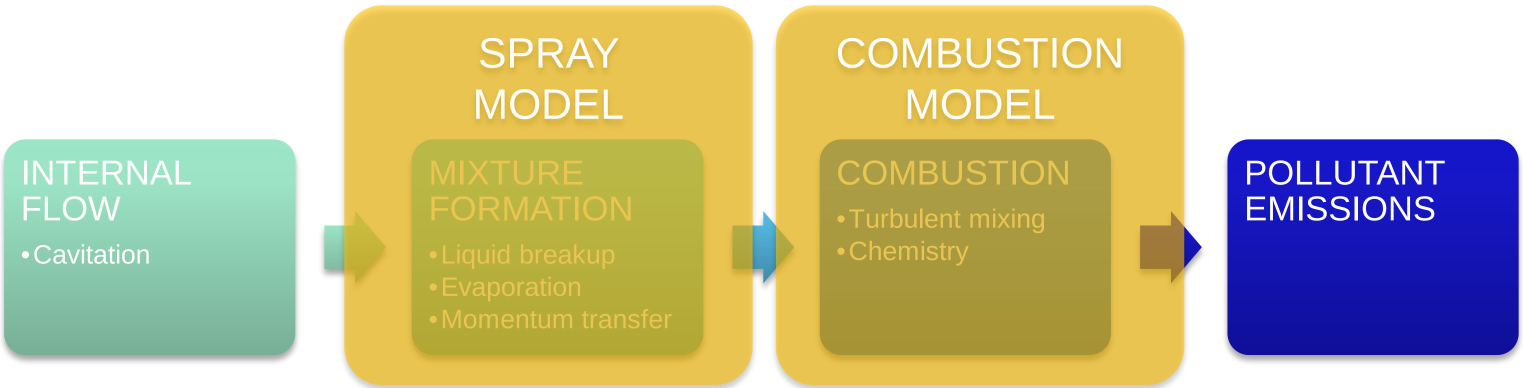
- Inert phase
  - Tip penetration (S)
  - Liquid stabilization (LL)
- Auto-ignition and diffusion flame
  - Tip penetration (S)
  - Ignition delay (t_{SoC})
  - Lift-off length (LOL)
  - Flame stabilization (FL)



BACKGROUND

CFD of combustion in Diesel engines still a challenge:

- Two fundamental modelling steps:



	SPRAY	COMBUSTION	TURBULENCE
CONVENTIONAL	LAGRANGIAN DDM	SIMPLIFIED KINETICS + TCI	RANS
ADVANCED	EULERIAN Σ-Y (diffuse interface)	DETAILED KINETICS + UFPV	RANS $\rightarrow$ LES

BACKGROUND

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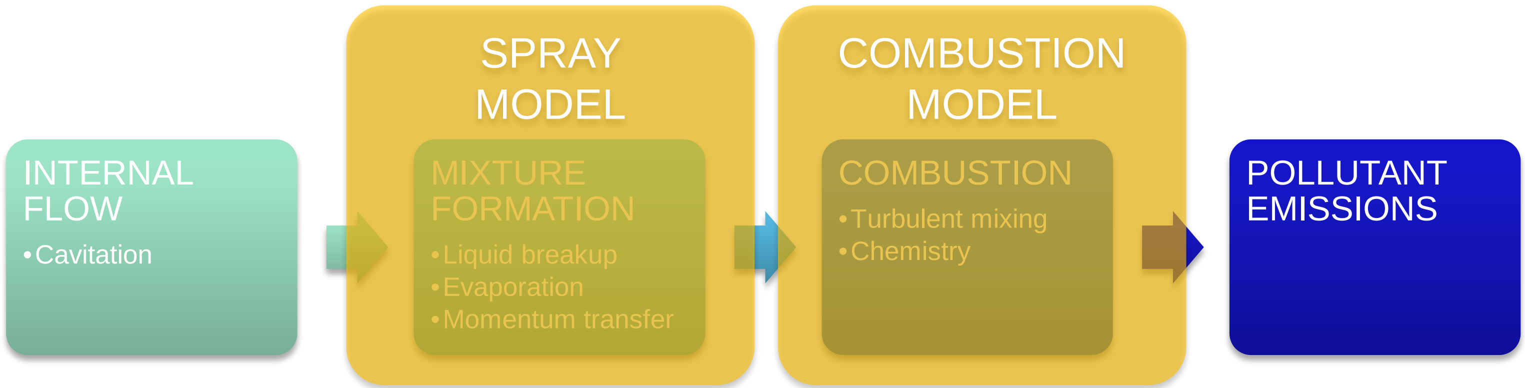

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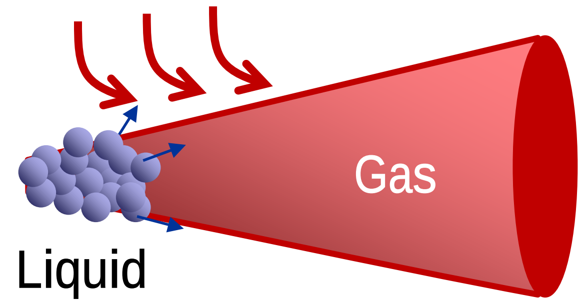
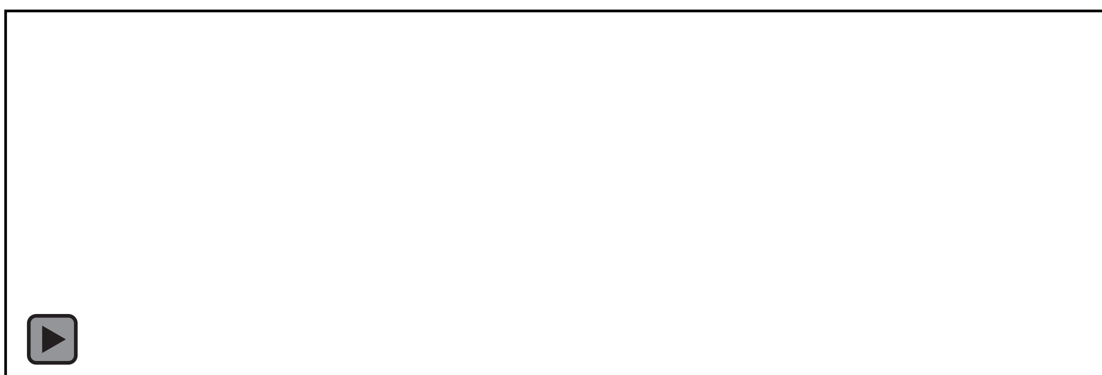
Eulerian spray modelling

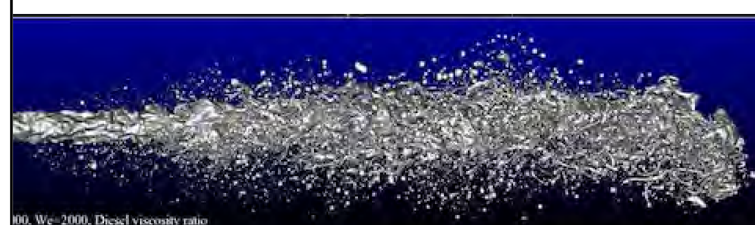
Motivation



- Classical spray DDM description
  - Liquid phase → lagrangian approach
  - Gas phase → eulerian framework
- Complex liquid-gas near-nozzle interface
  - Modeling *(and experiments)* should move away from the droplet concept within the spray dense core
  - DDM not well suited for this region
  - ICM unfeasible (↑↑ *Re* & *We)*

→ Diffuse-interface eulerian methods arises as an interesting option





Source: ECN, https://ecn.sandia.gov/

Source:https://ctflab.mae.cornell.edu/research.html

Eulerian spray modelling

Single-fluid diffuse-interface approach (Vallet & Borghi, AAS (2001))

- Flow scales separation at high *Re* & *We*
  - Large scale liquid dispersion independent from atomization processes occurring at smaller scales
- Mean velocity field
  - Liquid/gas mixture considered as a single velocity pseudo-fluid
- Liquid mass dispersion
  - Modeled as turbulent mixing of variable density fluid by means of liquid mass fraction (Y) transport eq.
- Atomization process
  - Mean liquid geometry modeled by surface area of the liquid-gas interphase (Σ)

$$\frac{1}{\overline{\rho}} = \frac{\tilde{Y}}{\rho_l} + \frac{1-\tilde{Y}}{\rho_g}$$

$$\frac{\partial \overline{\rho}\tilde{Y}}{\partial t} + \frac{\partial \overline{\rho}\tilde{u}_i\tilde{Y}}{\partial x_i} = -\frac{\partial \tau_i}{\partial x_i}$$

$$\frac{\partial \tilde{\Sigma}}{\partial t} + \frac{\partial \tilde{u}_j\tilde{\Sigma}}{\partial x_j} - \frac{\partial}{\partial x_j}\left(D_\Sigma \frac{\partial \tilde{\Sigma}}{\partial x_j}\right) = C_\Sigma \tilde{\Sigma}\left(1 - \frac{\tilde{\Sigma}}{\Sigma_{eq}}\right) + S_{\Sigma_{init}}$$

OF implementation

- Pressure eqn.

$$\nabla (U_p)_f = \nabla \cdot \phi^* - \nabla \cdot \left(\frac{1}{a_p} \nabla p \right)_f$$

Following Jasak's algorithm

$$\nabla \cdot (U_p)_f = -\frac{1}{\overline{\rho}} \frac{D\overline{\rho}}{Dt} = -\frac{1}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial \overline{p}} \frac{D\overline{p}}{Dt} - \frac{1}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial T} \frac{DT}{Dt} - \frac{1}{\overline{\rho}} \frac{\partial \overline{\rho}}{\partial \tilde{Y}} \frac{D\tilde{Y}}{Dt} - \frac{\overline{\rho}_{EOS} - \overline{\rho}}{\delta_t K_r \overline{\rho}}$$

Trask et al., JPP 28 (2012):685-693
García-Oliver et al., AAS 23 (2013):71–95

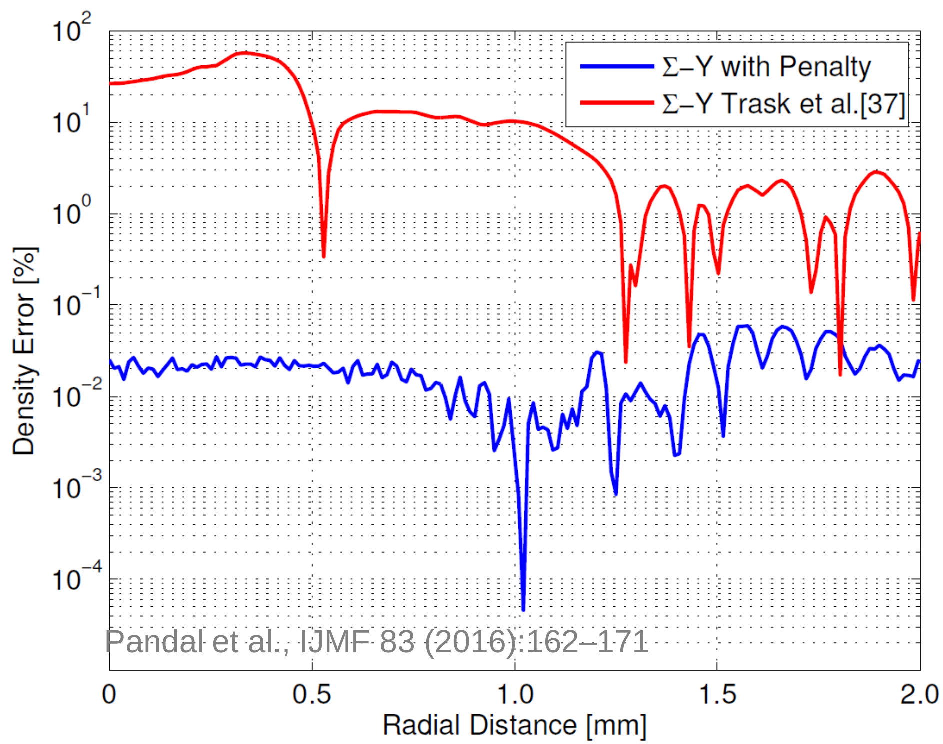
1. Compressibility effects.
2. Thermal expansion effects.
3. Multiphase mixing effects.
4. Relax penalty function

$\overline{\rho}_{EOS} \equiv$ From density equation

$\overline{\rho} \equiv$ From continuity

$\delta_t \equiv$ Time step

$K_r \equiv$ Constant multiplier



Pandal et al., IJMF 83 (2016):162–171

Eulerian spray modelling

Computational domain

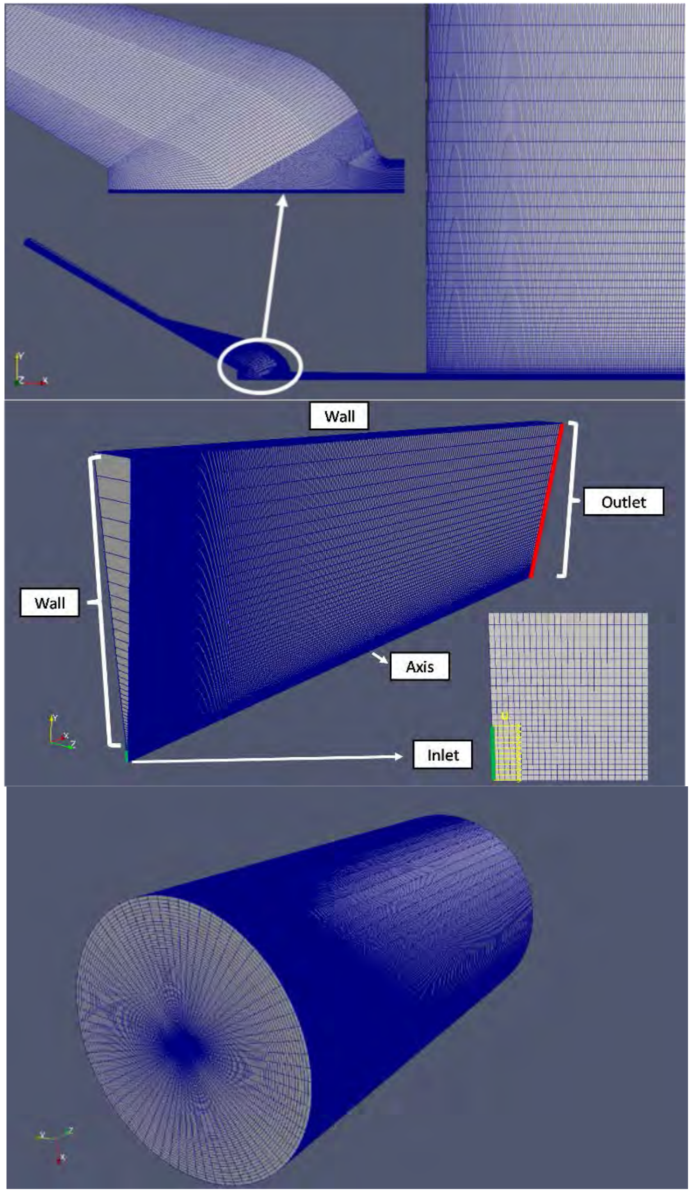
- Coupled and decoupled nozzle-spray flow simulations

Boundary conditions

- Bulk inj. velocity from MFR
- Non-reflecting at open-ends

Turbulence modelling

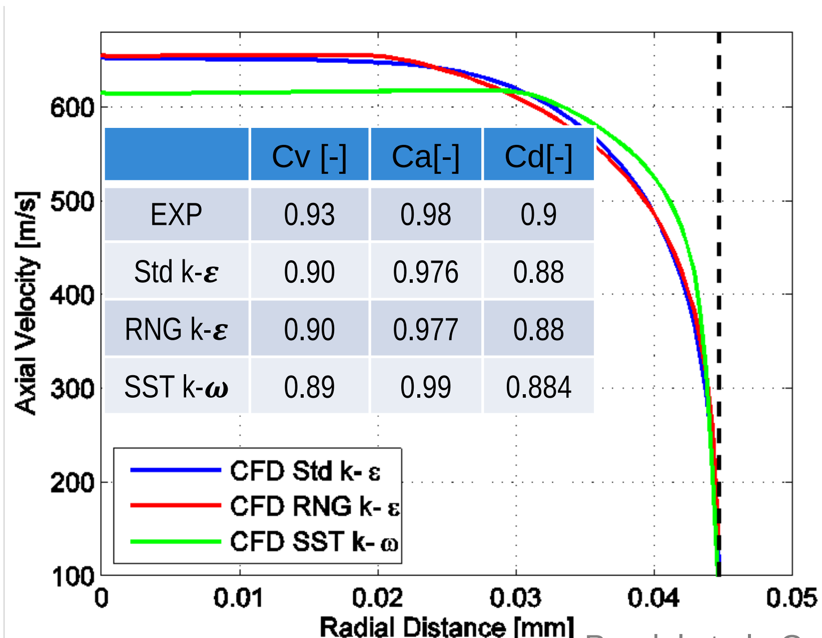
- RANS
  - Std & RNG k-ε
  - SST k-ω
- LES
  - Synthetic turbulent fluctuations at inlet
  - SGS model Sigma*



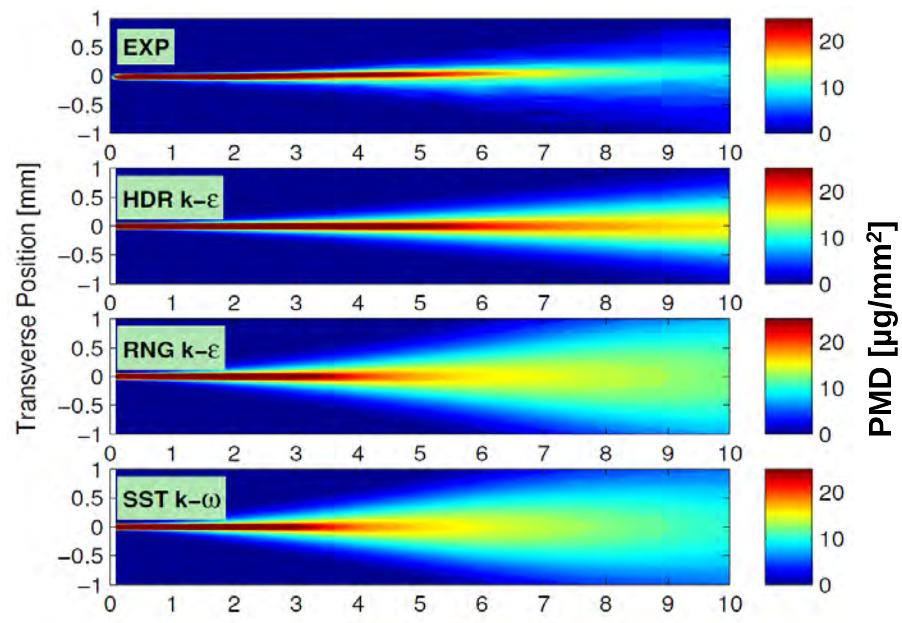
*Nicoud et al., POF 23(2011)

Near-field

- Turbulence modelling impact (RANS)
  - Nozzle outlet flow
    - – Sharper profile for *k-ω* (↑c_a) compared to *k-ε* models
  - Spray dispersion (PMD)
    - – Best results for *Std k-ε* +$c_{1\varepsilon}$=1.6, radial dispersion overpredicted by RNG and *k-ω*



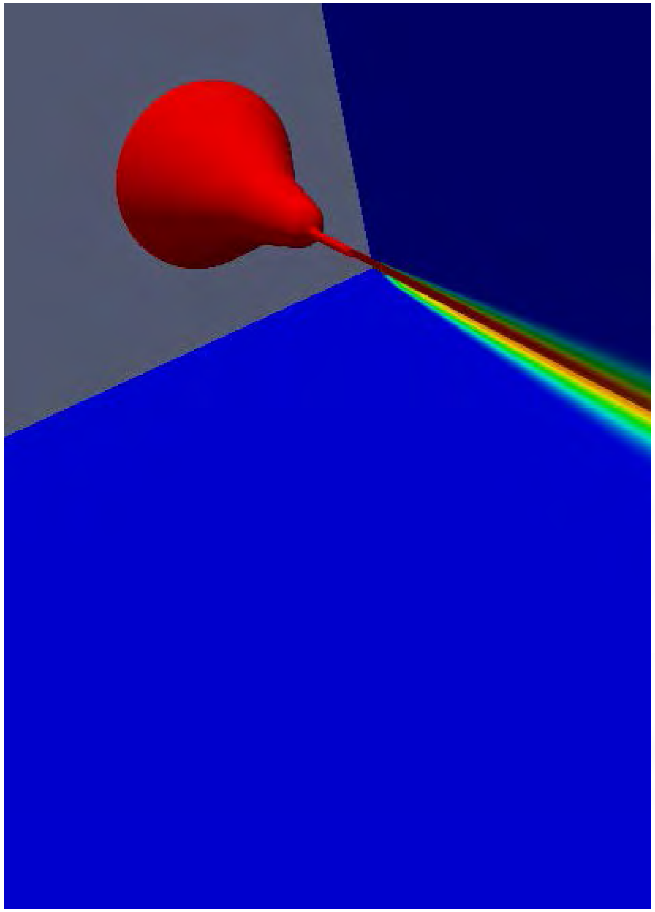
	Cv [-]	Ca[-]	Cd[-]
EXP	0.93	0.98	0.9
Std k-ε	0.90	0.976	0.88
RNG k-ε	0.90	0.977	0.88
SST k-ω	0.89	0.99	0.884

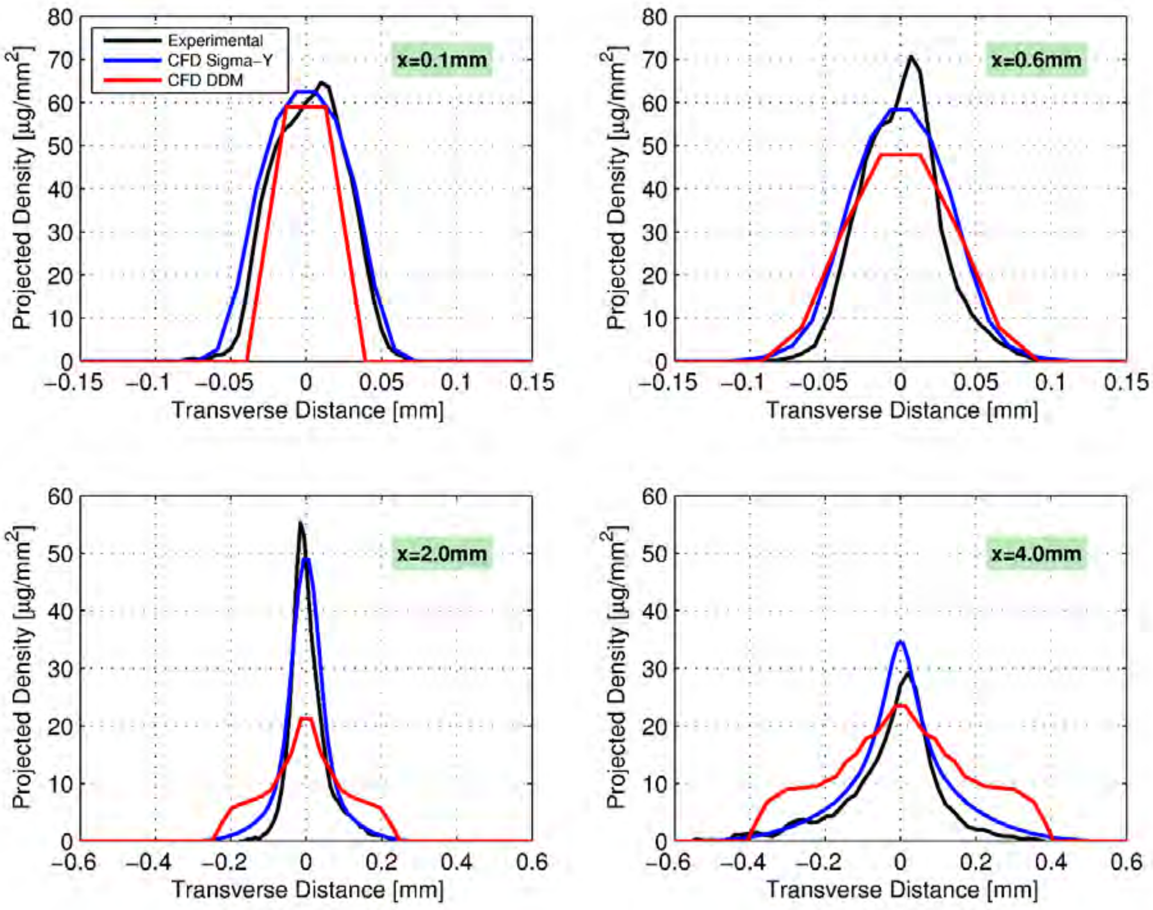


Pandal et al., CompFluid 157(2017):9-20

Near-field

- Improved near-nozzle liquid dispersion compared to DDM



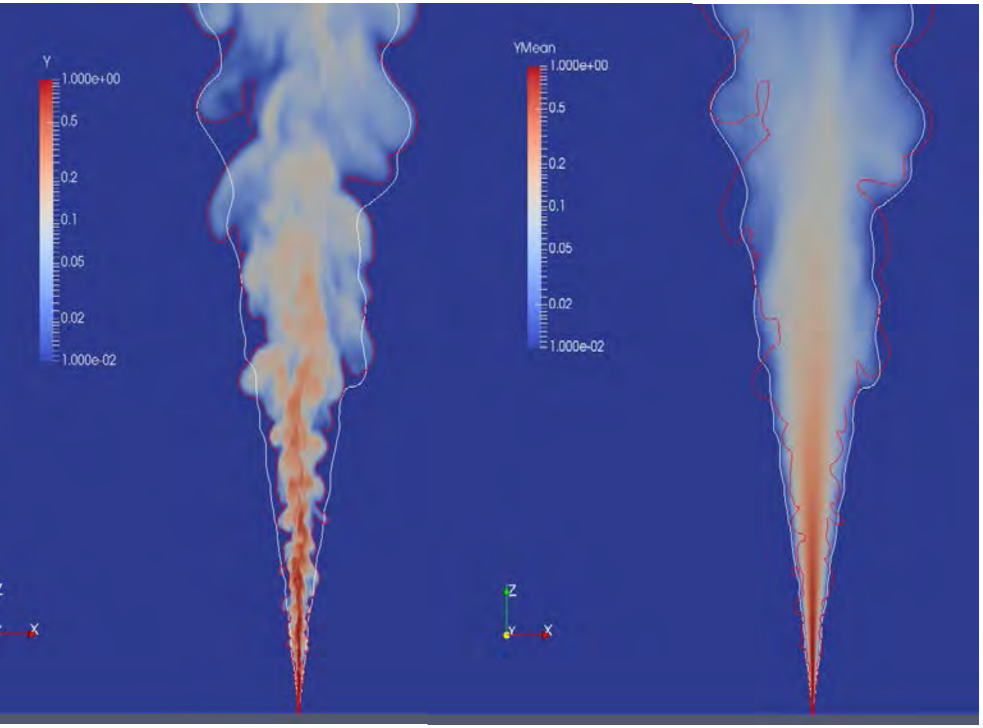


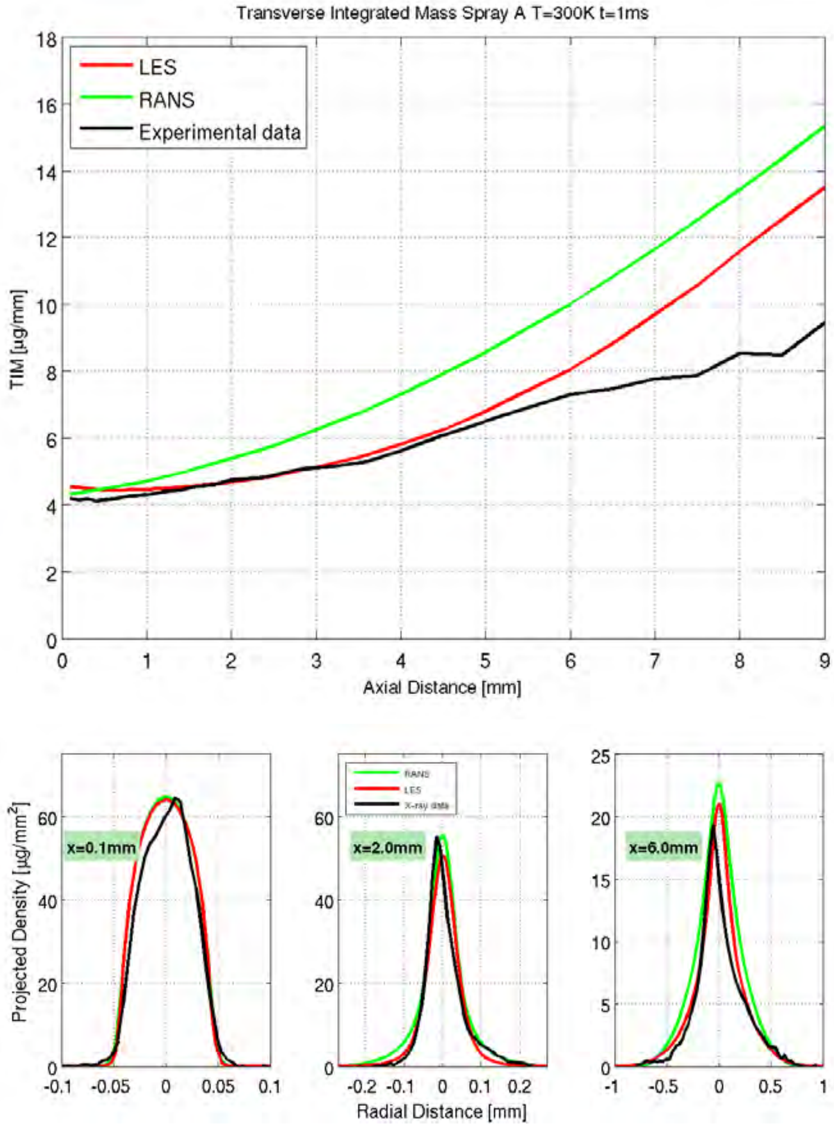
Desantes et al., AAS 26 (2016):713-737

Eulerian spray modelling

Near-field

- RANS→LES
  - TIM shows the potential of less diffusive LES modelling



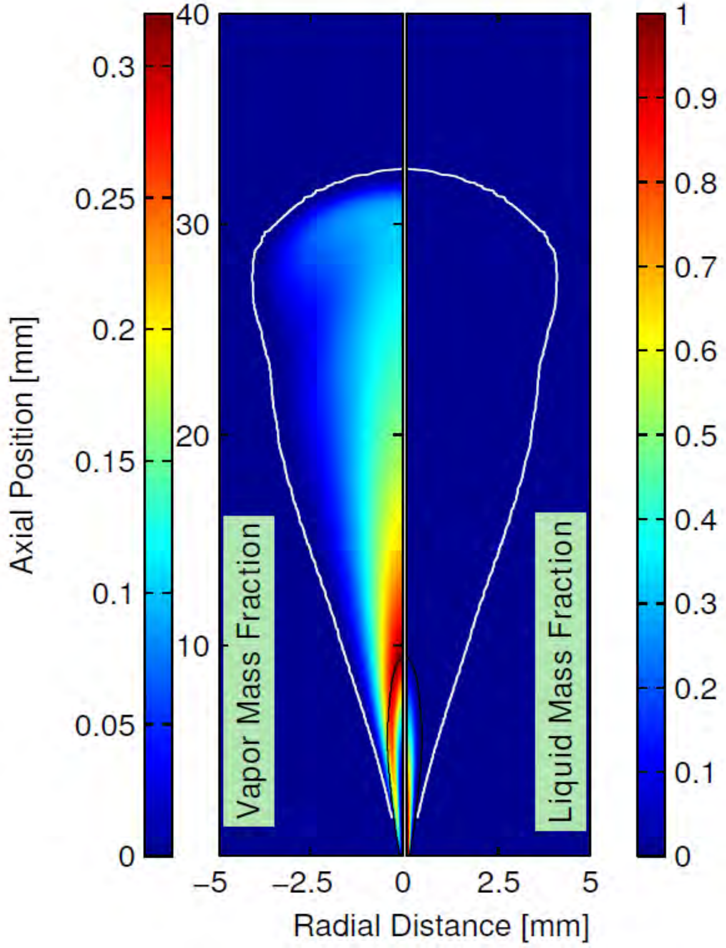


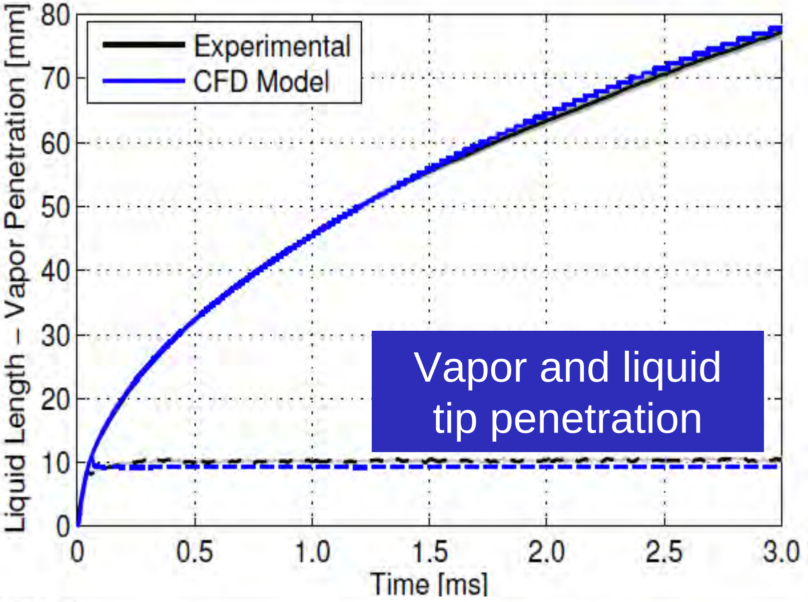
Desantes et al., ILASS Europe (2017)

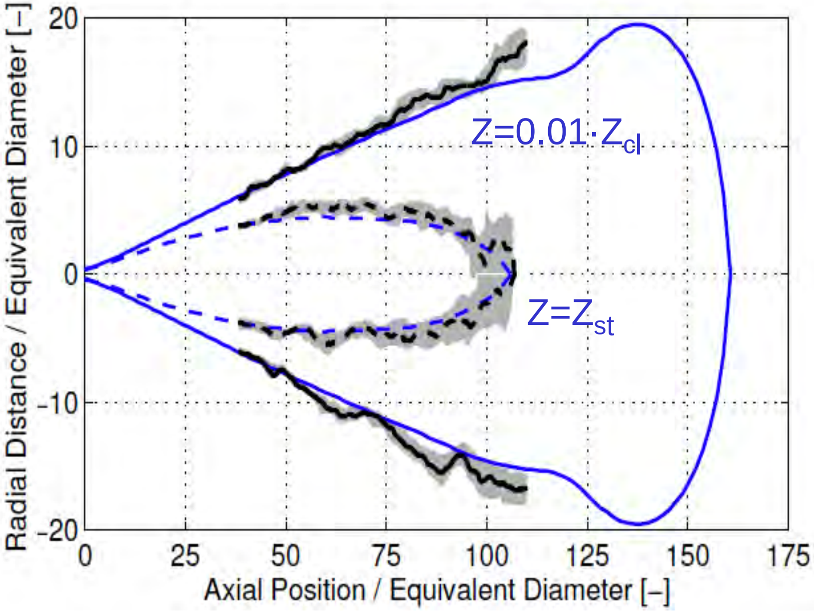
Eulerian spray modelling

Far-field

- Consistent results downstream



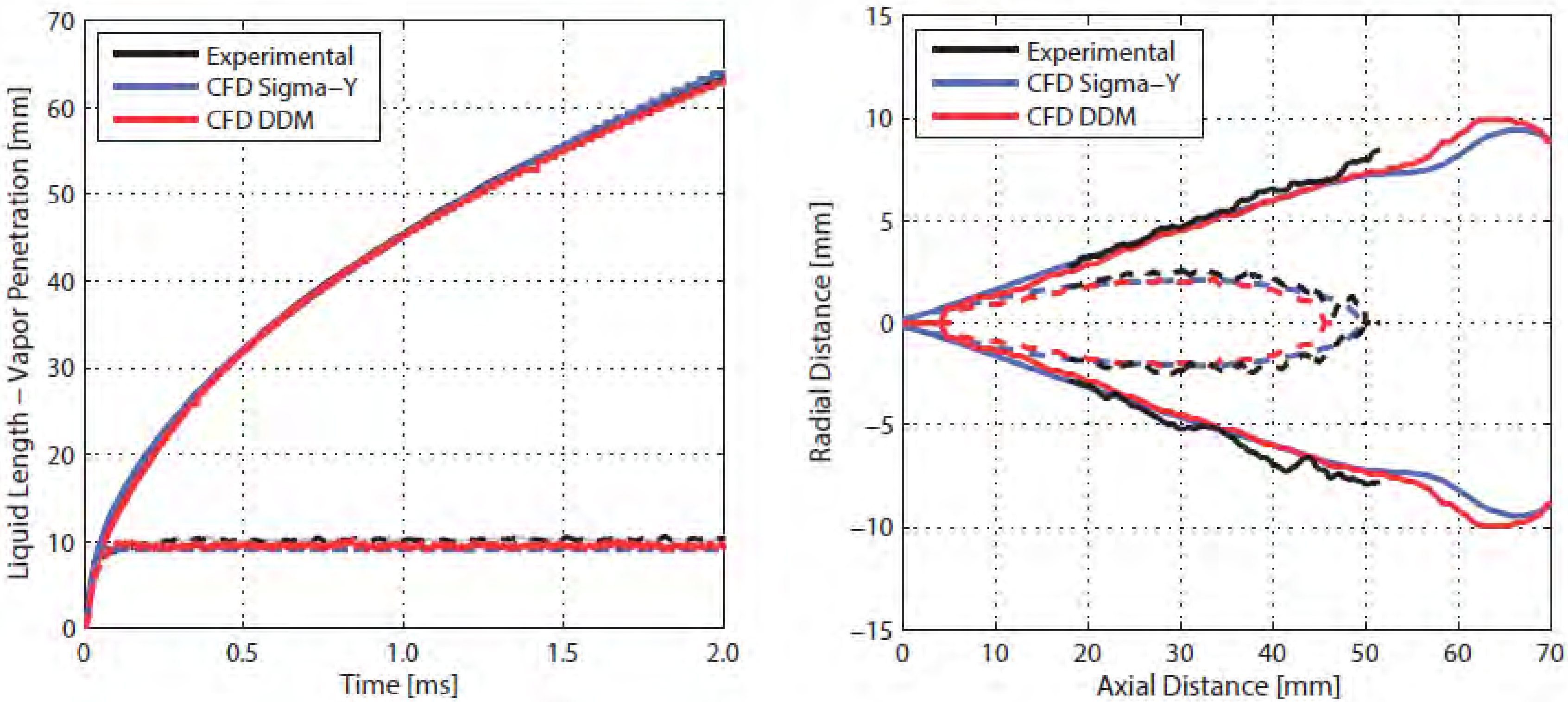




García-Oliver et al., AAS 23 (2013):71–95

Far-field

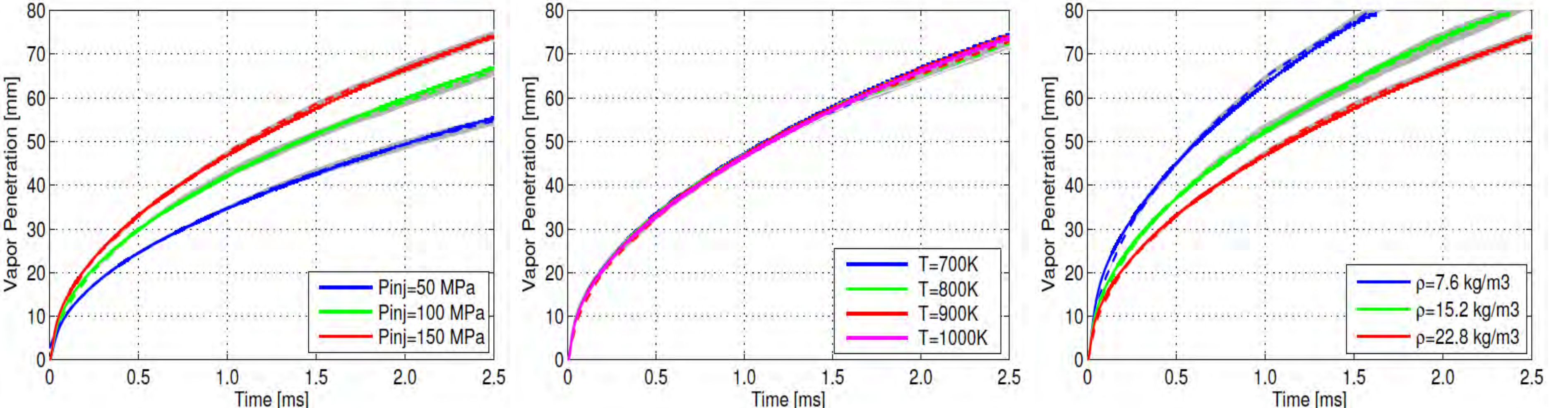
- Improved predictions compared to calibrated DDM



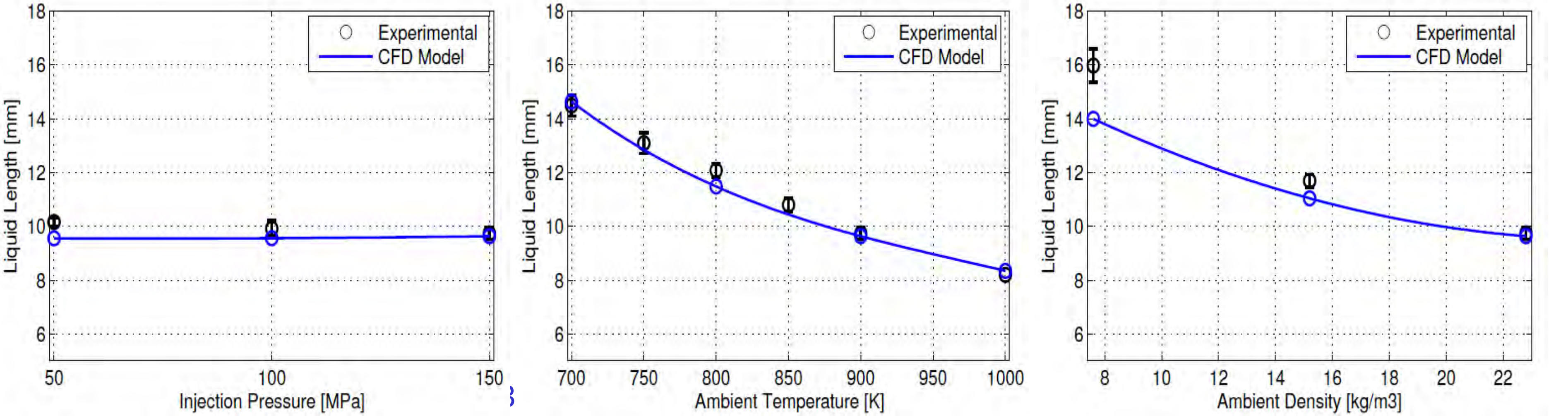
Desantes et al., AAS 26 (2016):713-737

Eulerian spray modelling

Far-field: Parametric variations



Injection Pressure | Ambient Temperature | Ambient density



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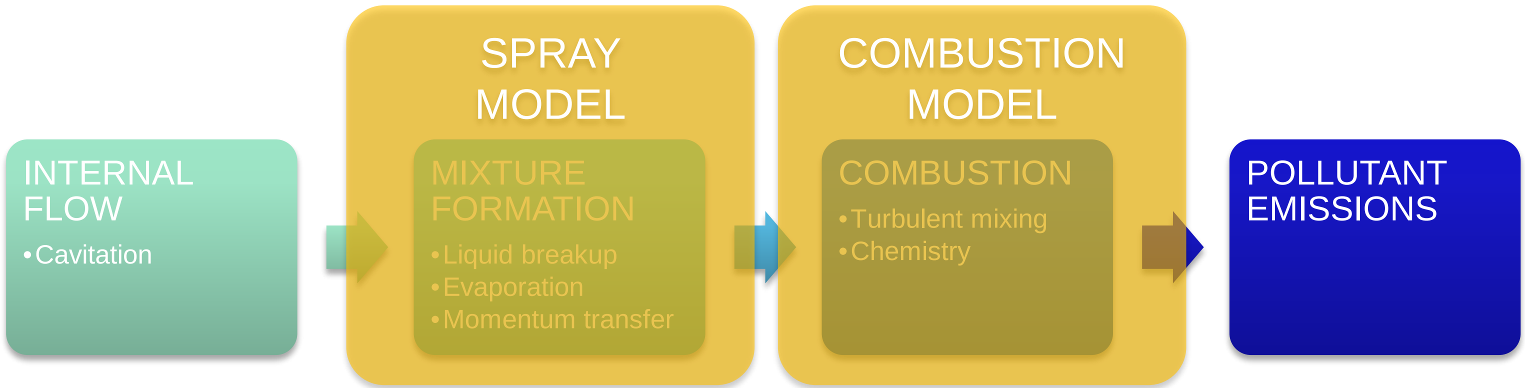

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Approach

- Unsteady Flamelet Model (USFM)

  (Naud et al, CAF, 2014)

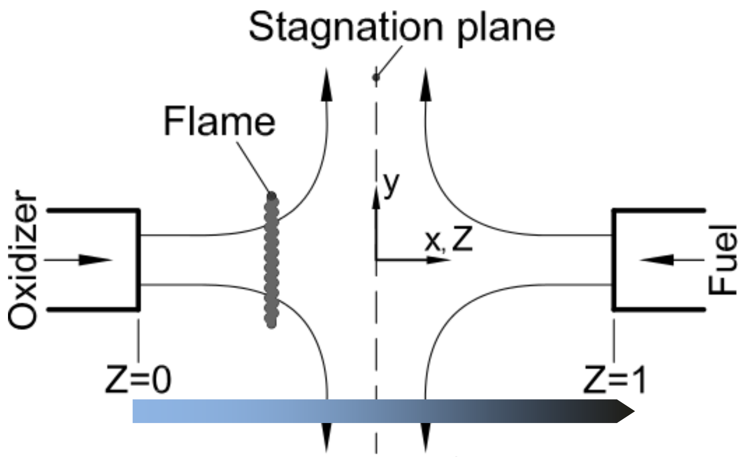
- Tabulated chemistry → Large chemical mechanisms

- **A**pproximated **D**iffusion **F**lamelet → In order to reduce the computational effort required to generate the laminar flamelets database

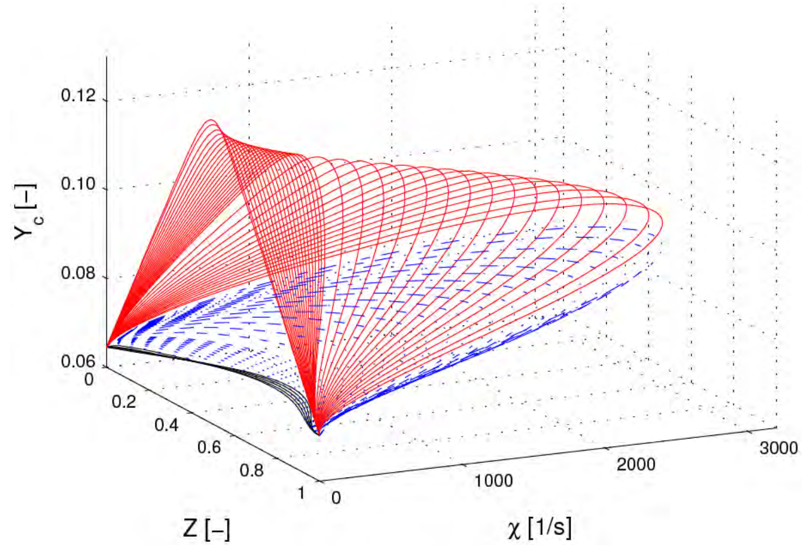
  - Source terms from a set of HR
  - Laminar diffusion accounted later by solving the flamelet equation ONLY for the progress variable

- Currently moving to fully detailed Flamelet calculations (DF)

  (Payri et al., AppMathModel, 2017)



$$\rho \frac{\partial \psi_i}{\partial t} = \rho \frac{\chi}{2} \frac{\partial^2 \psi_i}{\partial Z^2} + \dot{\omega}_i$$



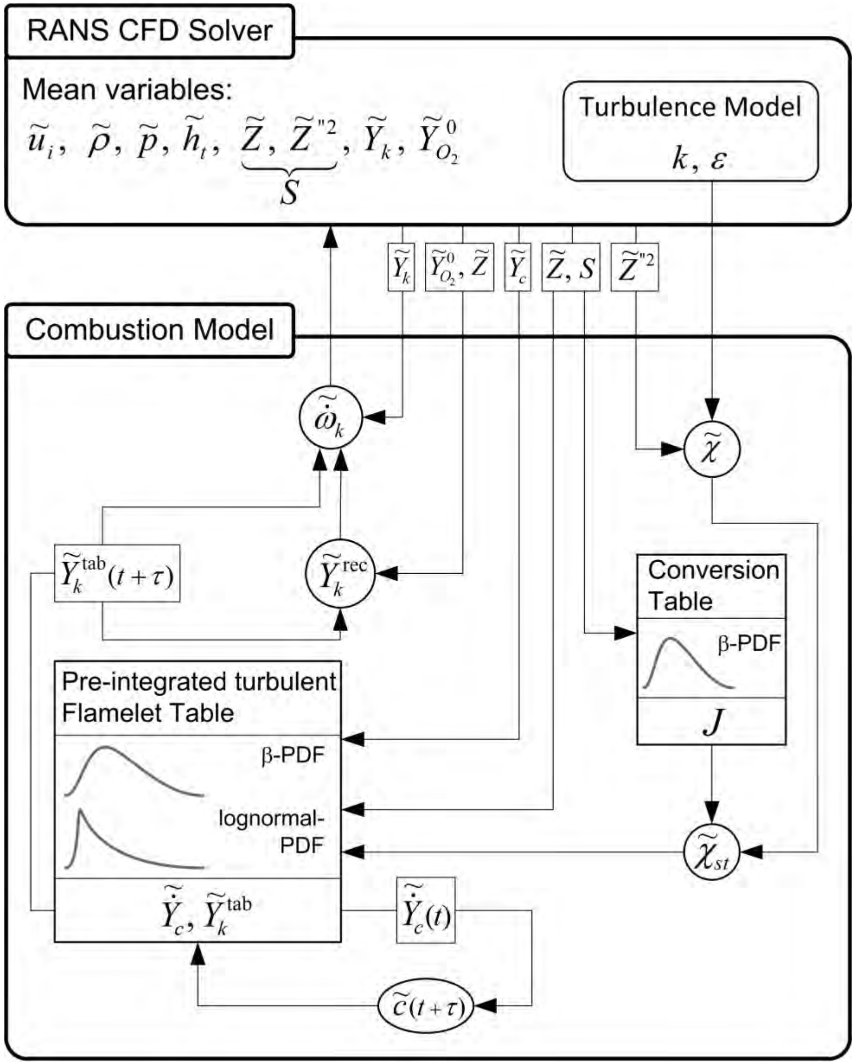
COMBUSTION MODEL

Approach

- TCI accounted by presumed-PDF (PCM)
  - Beta-PDF for mixture fraction
  - LogNormal-PDF for SDR (χ)
- Coupling with CFD by transporting a set of control variables + key species
  - $\tilde{Z}$, $\tilde{Z}''^2$, $\tilde{Y}_k$
  - Algebraic model for $\tilde{\chi}_{st}$

$$\tilde{\chi} = C_\chi \frac{\varepsilon}{k} \tilde{Z}''^2$$

$$\tilde{\chi} = \tilde{\chi}_{st} \int_{[Z]} \frac{F(z)}{F(z_{st})} P^{\beta}_{\tilde{Z},\tilde{Z}''^2}(z)\, \mathrm{d}z = \tilde{\chi}_{st}\, J\left(\tilde{Z}, S\right)$$

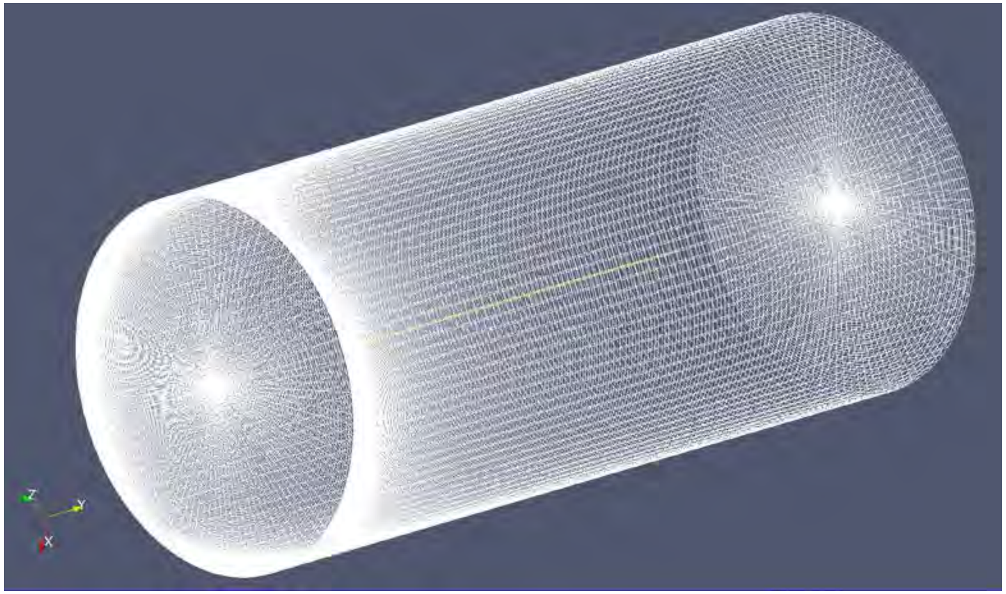


Winklinger, J., Ph.D. Thesis (2014)

SPRAY COMBUSTION

Modeling setup

- Domain (ϕ54x108 mm)
  - *RANS:* std k-ε + $C_{1\varepsilon}$=1.55
    - 2D axsym (50 kcells)
    - Min cell size 250 μm
  - *LES:* dynamic Structure*
    - 3D (3.6 Mcells)
    - Min cell size 62.5 μm



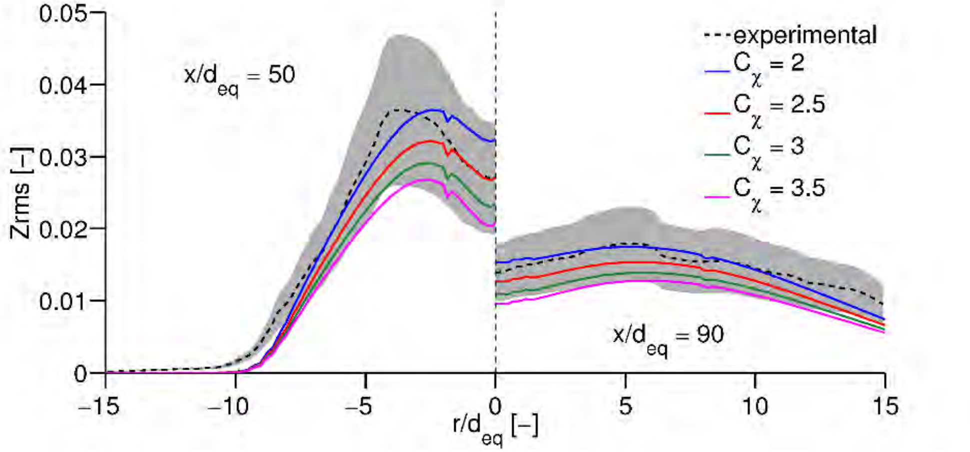
- Chemical mechanisms:
  - Narayanaswamy et al, Comb.Flame 2014
    - 255 species
  - Yao et al, Fuel, 2017
    - 54 species
  - Wang et al, Fuel, 2014
    - 100 species

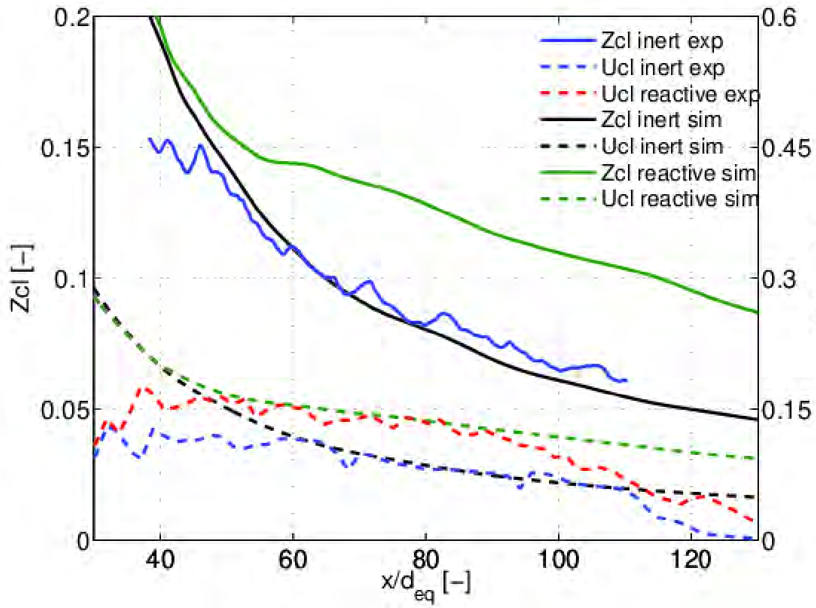
- DDM spray:
  - KH + RT atomization & break-up

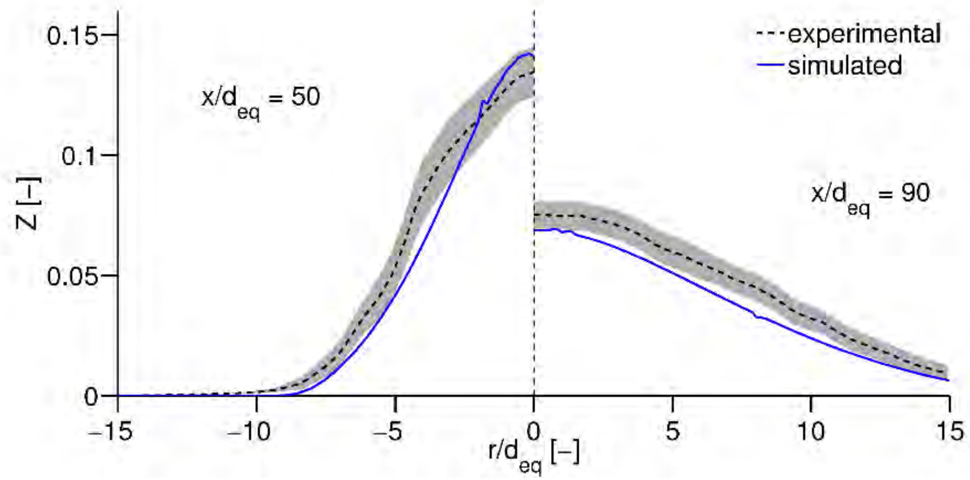
*Pomraining & Rutland, AIAA 40 (2002)
Bharadwaj et al. IJER 10(2009)

Spray calibration & assessment

- Necessary step to capture mixing field:
  - Fair agreement of averaged fields with RANS
  - Fluctuations are captured with typical calibration constant value



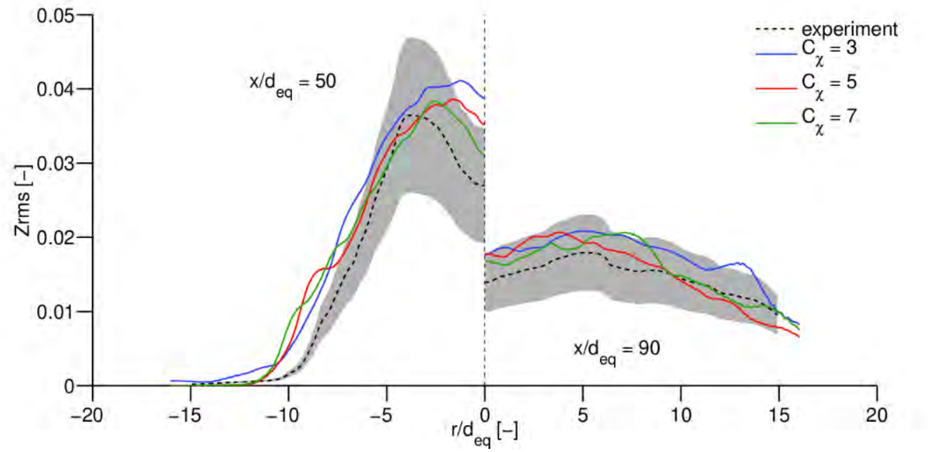


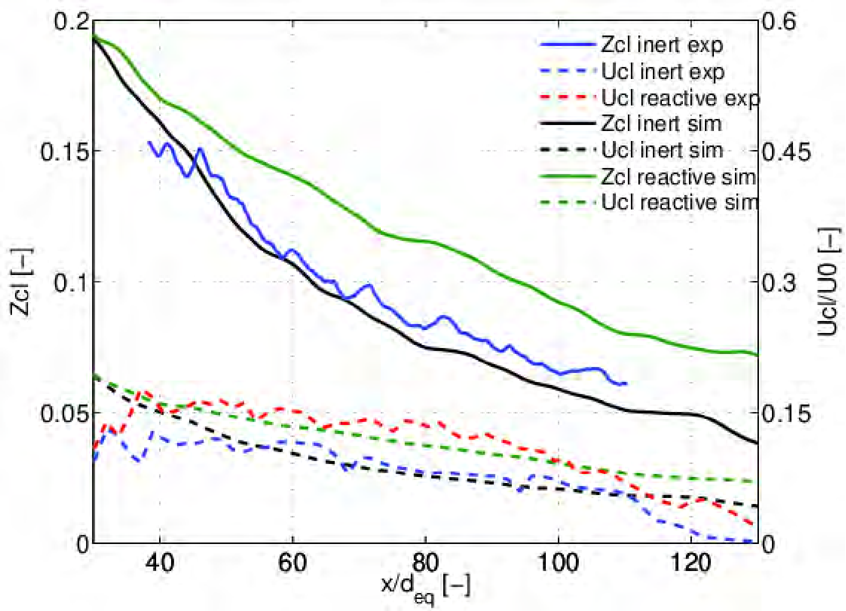


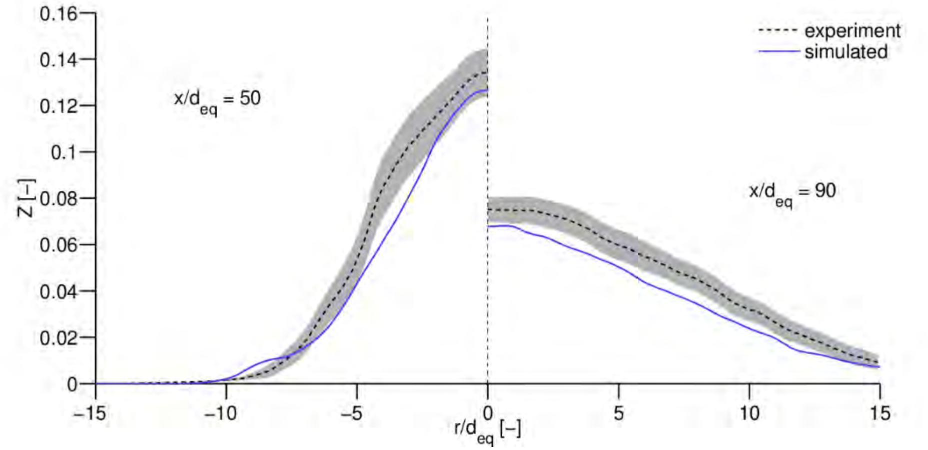
Desantes et al., Applied Thermal Engineering 117 (2017): 50–64

Spray calibration & assessment

- Necessary step to capture mixing field:
  - LES provides good averaged values and lower model constant impact on fluctuations





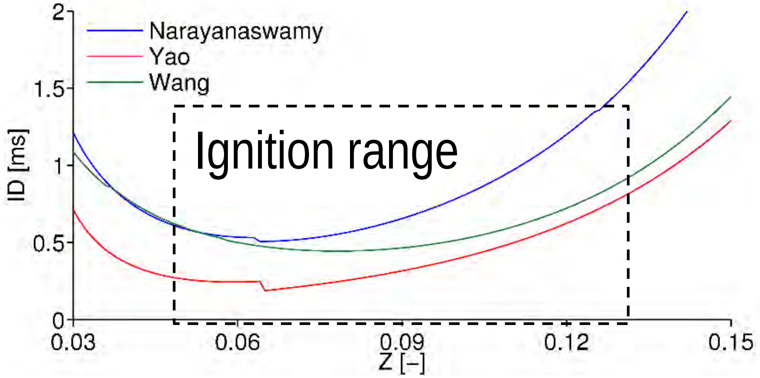


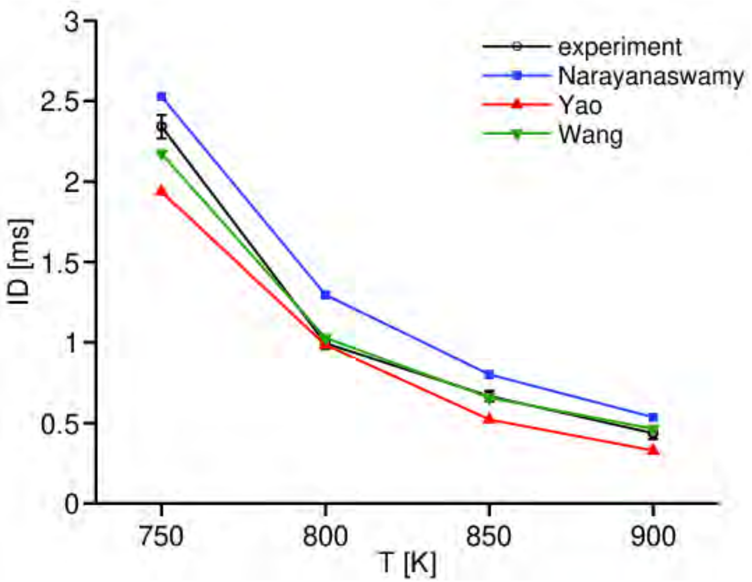
COMBUSTION MODEL

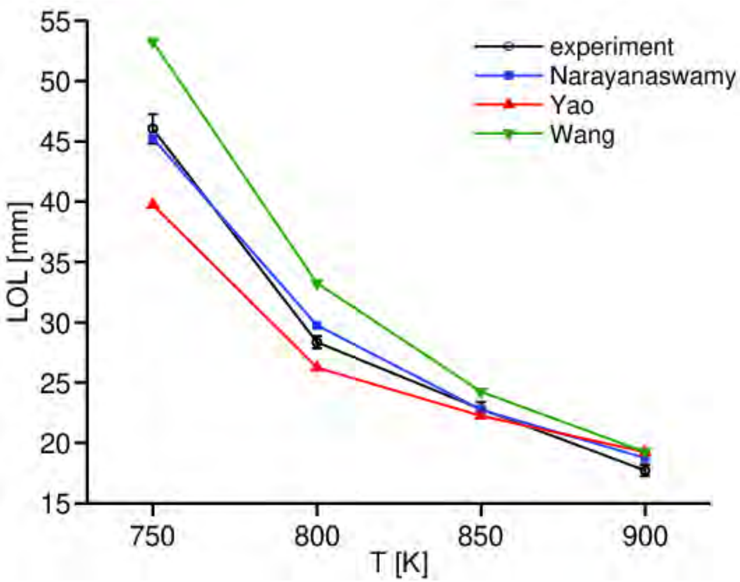
Global combustions indicators

- ID: Central role of chemistry
  - Similar sensitivity in sprays as in homogeneous conditions
- LOL: TCI problem
  - Both flow and chemistry accounts…

HRs calculation



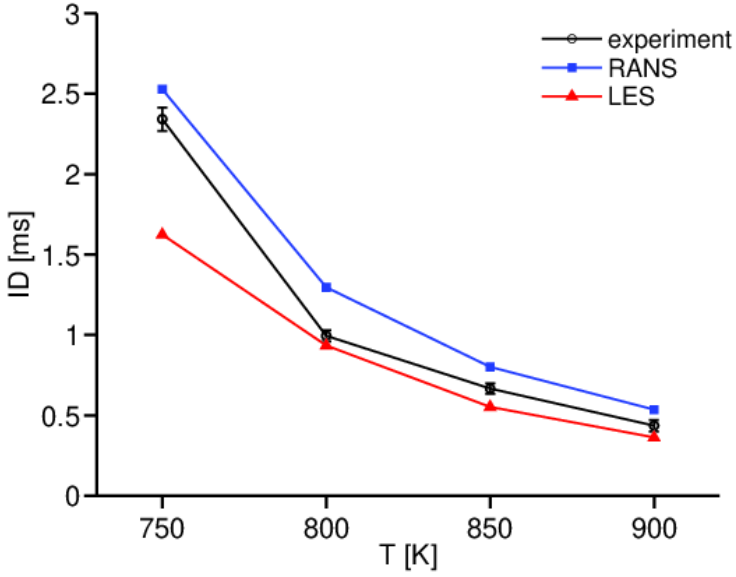


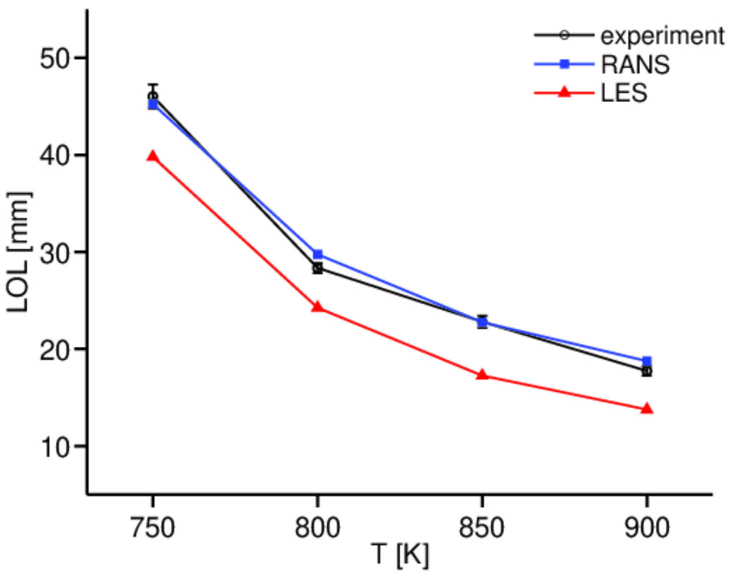


Desantes et al., ILASS (2017): 50–64

Global combustions indicators: RANS → LES

- Both ID and LOL predictions are affected by turbulence modelling approach
  - ➢ID is noticeably decreased
  - ➢LOL is also shortened

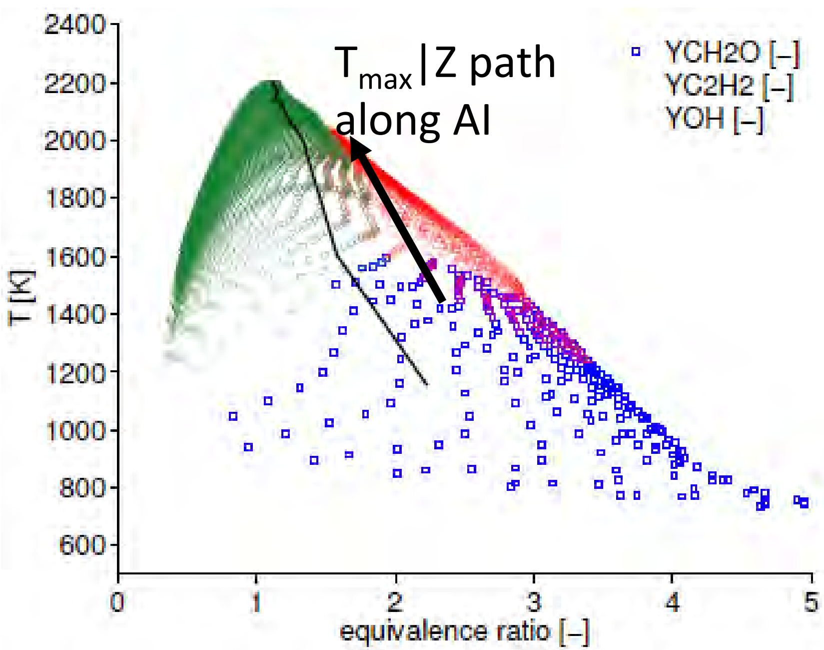


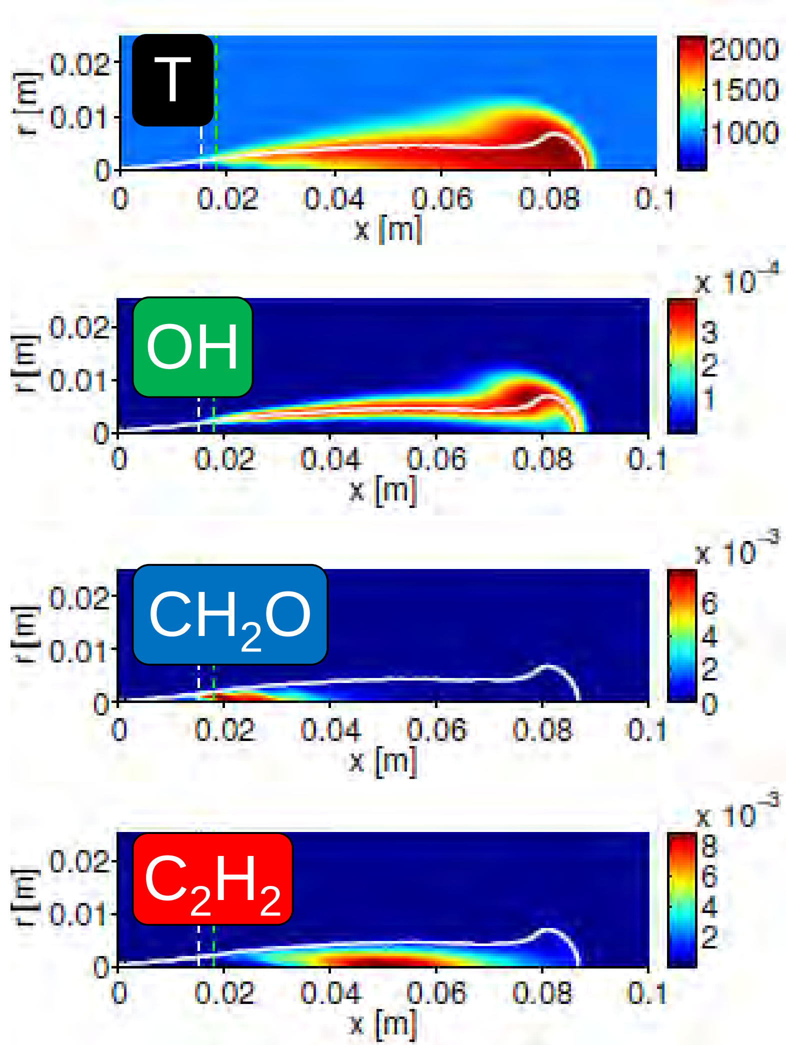


Narayanaswamy Chemical mech.

Flame structure

- RANS simulations produce meaningful flame structure with the proposed approach



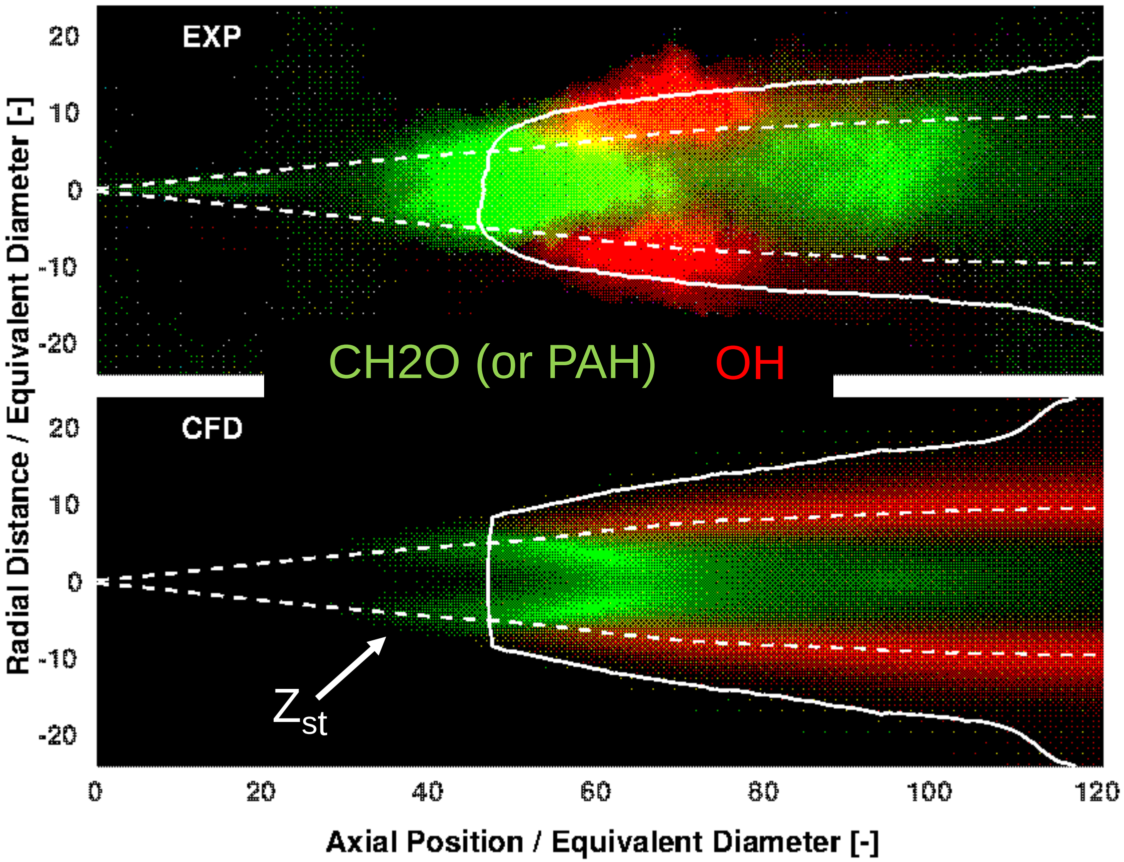


Desantes et al. / Applied Thermal Engineering 117 (2017) 50–64

COMBUSTION MODEL

Flame structure

- Further validation require refined experimental diagnostics

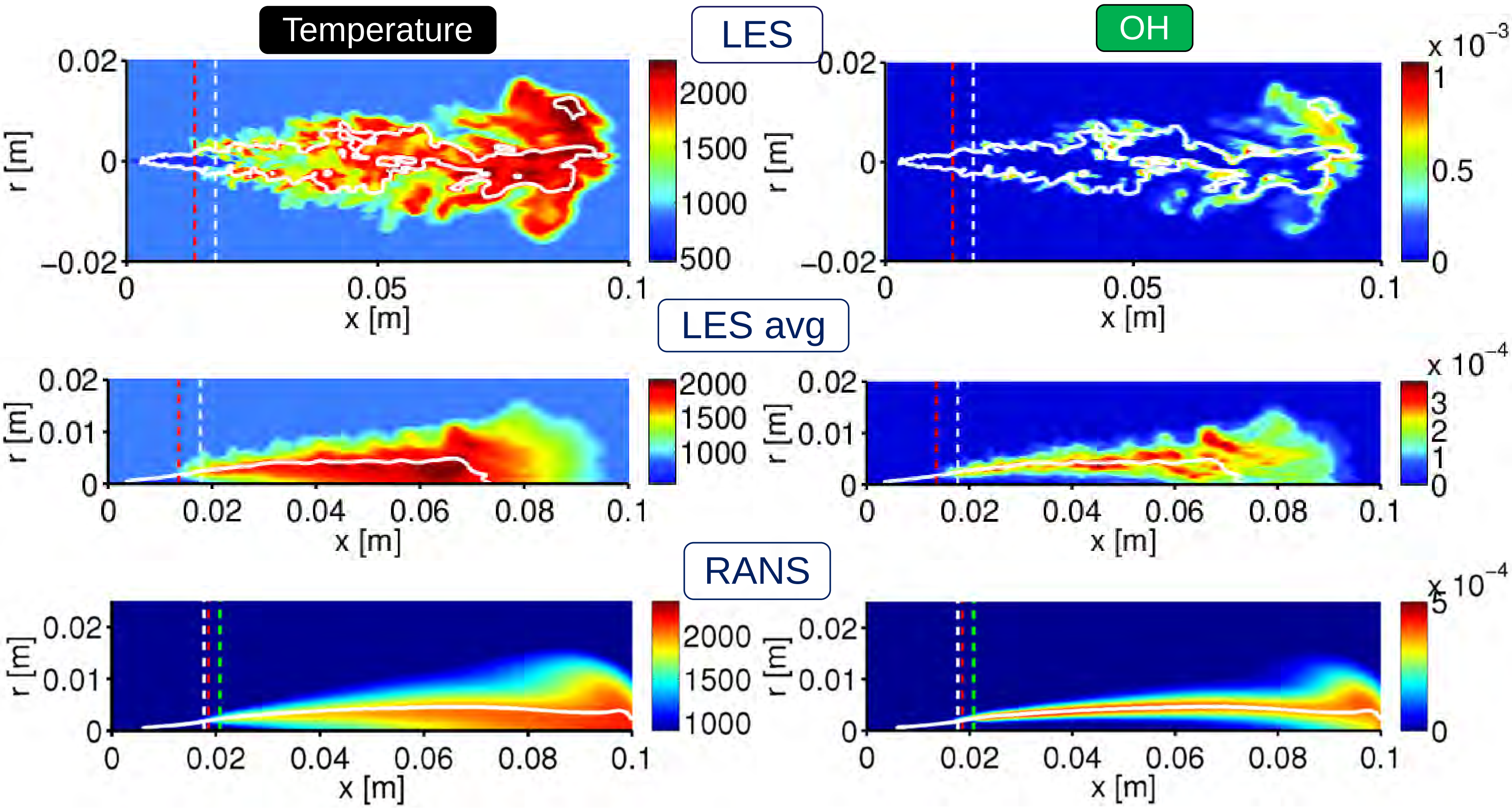


Pandal et al., IJMF 99 (2018):257–272

COMBUSTION MODEL

Flame structure

- RANS → LES



Flame structure

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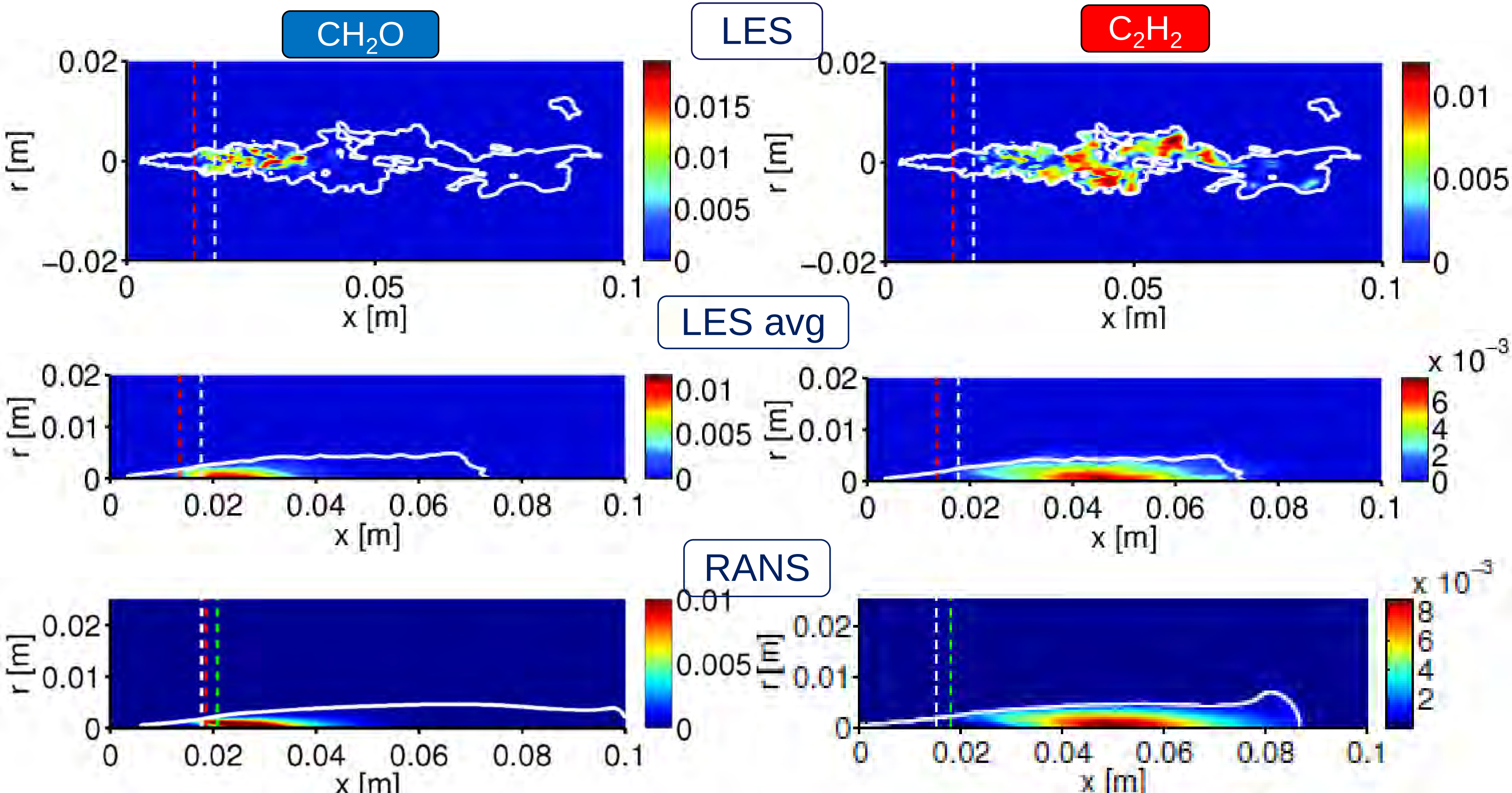
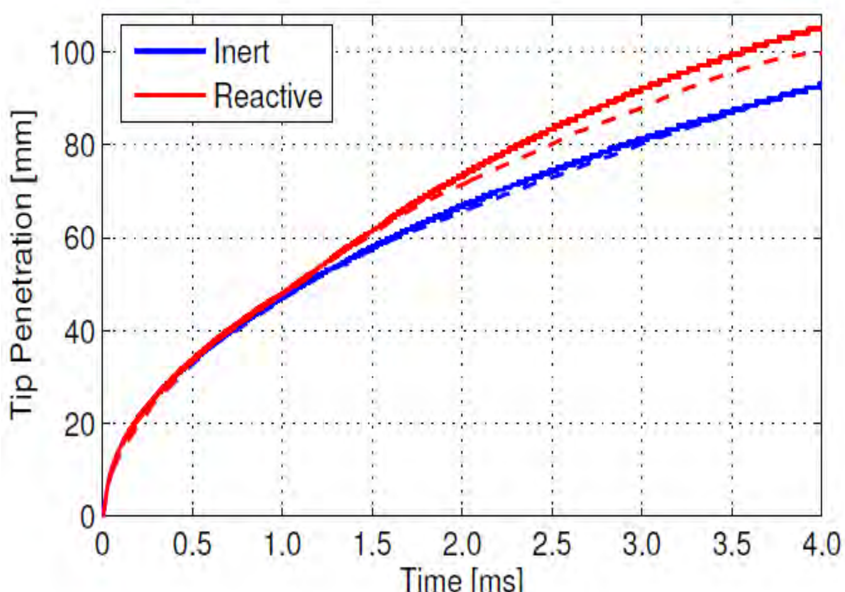


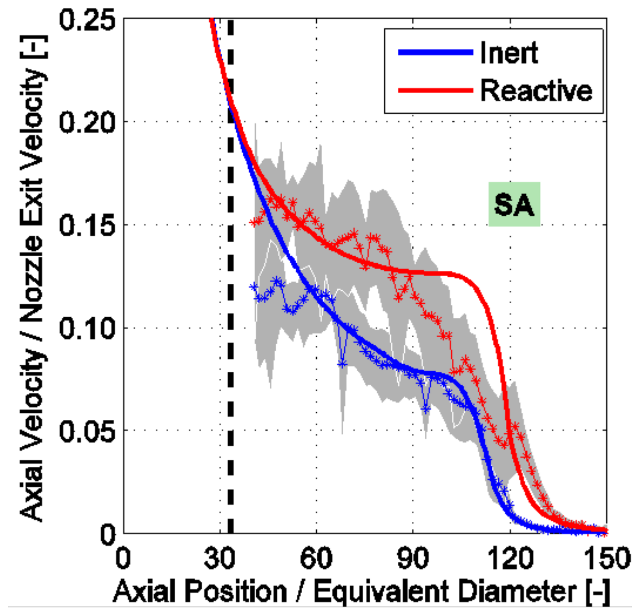
CONCLUSIONS

On-going work

- Pollutant (NOx-Soot) integration in UFPV model
- Coupled spray and combustion models

	SPRAY	COMBUSTION	TURBULENCE
CONVENTIONAL	LAGRANGIAN DDM	SIMPLIFIED KINETICS + TCI	RANS
ADVANCED	EULERIAN Σ-Y	DETAILED KINETICS + UFPV	RANS → LES





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Thanks for your attention !