Modelling of soot production (and radiation) in large eddy simulation of lab-scale pool fires

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INTRODUCTION

- **Strong collaboration between AMU and EDF R&D**
- **Objective: High fidelity modelling of fire flames**
  - Fluid dynamics: natural convection, buoyancy
  - Well and under-ventilated combustion
  - Radiative transfer is the dominant mode of heat transfer
  - Soot production
  - All these processes taking place in a turbulent flow

- **Interaction flow/chemistry/radiation/soot/turbulence**

- **Phd Thesis Antoine BOUFFARD**

- **Outlines**
  - Numerical model
  - Soot production model and soot production/turbulence interaction
  - Results and discussions
  - Conclusions

Essai-Heptane, IGNIS - EDF

NUMERICAL MODEL

LES

- Filtered NS equation + transport equations for $\tilde{h}$, $\tilde{Z}$ and $\widetilde{Z^2}$
- SGS momentum stresses and scalar fluxes: dynamic Smagorinsky and eddy diffusivity models

Combustion model

- Non-adiabatic flamelet: $\phi_g(Z, \chi, X_R)$
- Flamelet library (Ethylene: Qin et al. (2000), Heptane: KM1 (2012))
- Filtered thermochemical quantities: Presumed FDF Closure
  - Z, χ and X_R: statistically independent
  - β-distribution for Z and δ-distributions for χ and X_R: $\tilde{\phi} = \int_0^1 \phi_g(Z, \tilde{\chi}, \widetilde{X_R})\beta(Z; \tilde{Z}, \widetilde{Z''^2})\, dZ$
  - $\widetilde{Z''^2} = \widetilde{Z^2} - \tilde{Z}^2$
  - $\tilde{\chi} = \frac{(\tilde{D} + D_T)}{C_I \Delta^2} \widetilde{Z''^2}$

Radiation model

- Radiating species: CO_2, H_2O, Fuel vapour, soot
- Gas radiative property model: RCFSK (Solovjov et al., JQSRT 2018)
- Emission TRI: Presumed FDF Closure
- Absorption TRI: OTFA ($\overline{\kappa_i I_i} = \overline{\kappa_i}\, \overline{I_i}$)

SOOT MODELLING

- Soot model
  - 2-equation C_2H_2/C_6H_6-based model (Lindstedt, 1994) : Transport of $\tilde{Y}_s$ and $\tilde{N}_s$
  - Soot processes: nucleation, surface growth, oxidation by O_2 and OH, coagulation

- SGS soot/turbulence interaction
  - Transport equation for $\widetilde{N_s^2}$
  - Soot production reaction rate : Closure

$$\bar{\dot{\omega}} = \bar{\rho} \int \frac{1}{\rho^{fl}(\phi_g)} \dot{\omega}(\phi_g, \phi_s) P(\phi_g, \phi_s)\, d\phi_g d\phi_s \quad = \bar{\rho} \int \frac{1}{\rho^{fl}(\phi_g)} \dot{\omega}(\phi_g, \phi_s) P(\phi_s|\phi_g) P(\phi_g)\, d\phi_g d\phi_s$$

$$\phi_g = \{Z, \chi, X_R\} \qquad \phi_s = \{Y_s, N_s\}$$

$$P(\phi_g) = \tilde{\beta}(Z; \tilde{Z}, \widetilde{Z''^2})\delta(\chi - \tilde{\chi})\delta(X_R - \widetilde{X_R})$$

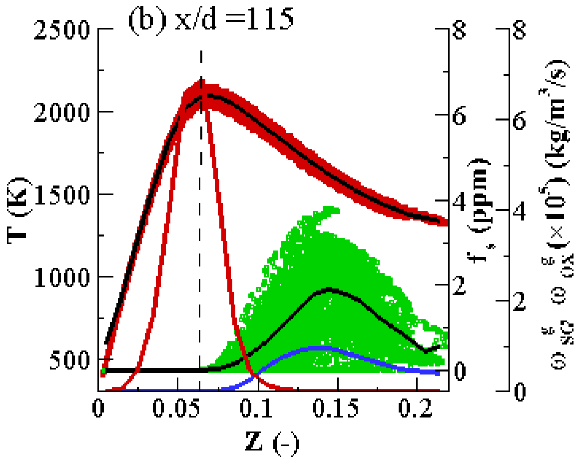
  - Determination of $P(\phi_s|\phi_g)$

SOOT MODELLING

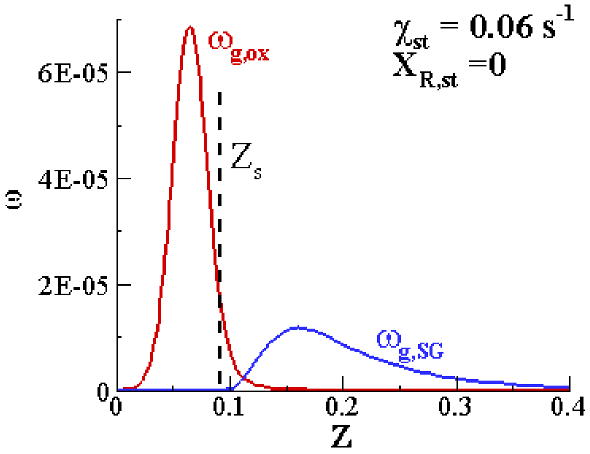
- Two FDF are designed to account for two main features of soot production process at the SGS
  - M_2: Spatial intermittency (Mueller & Pitsch, 2012)

$$P(\phi_s|\phi_g) = [\alpha\delta(\phi_s) + (1-\alpha)\,\delta(\phi_s - \phi_s^*)]$$

  - M_1 : Soot oxidation fast chemistry (Yang et al., 2019)
  - ✓ Z-space: Soot does not exist over the entire region of soot oxidation
  - ✓ Soot quantities: correlated with mixture fraction



$$P(\phi_s|\phi_g) = \alpha\delta(\phi_s) + (1-\alpha)\delta[\phi_s - \phi_s^* H(Z - Z_s)]$$



✓ Assumption: soot burns as soon as it ceases to be produced Z_s → location where C_2H_2 is completely consumed

RESULTS AND DISCUSSIONS

- **15-kW buoyant ethylene turbulent diffusion flames (FM Global)**
  - X_{O2} = 0.21; 0.168; 0.152
  - Inner D = 13.7 cm
  - SVF statistics: LII (Xiong et al., C&F 2021)
  - Temperature: Dual thermocouple technique (Ren et al., Fire Safety 2021)
  - Radiation characteristics (Zeng et al, PROCI 2019)

- Computational details
  - Simulation time 50s, Δt=0.5ms
  - Domain: $3 \times 3 \times 1.5\ m^3$ with minimal size cell of 2.5 mm

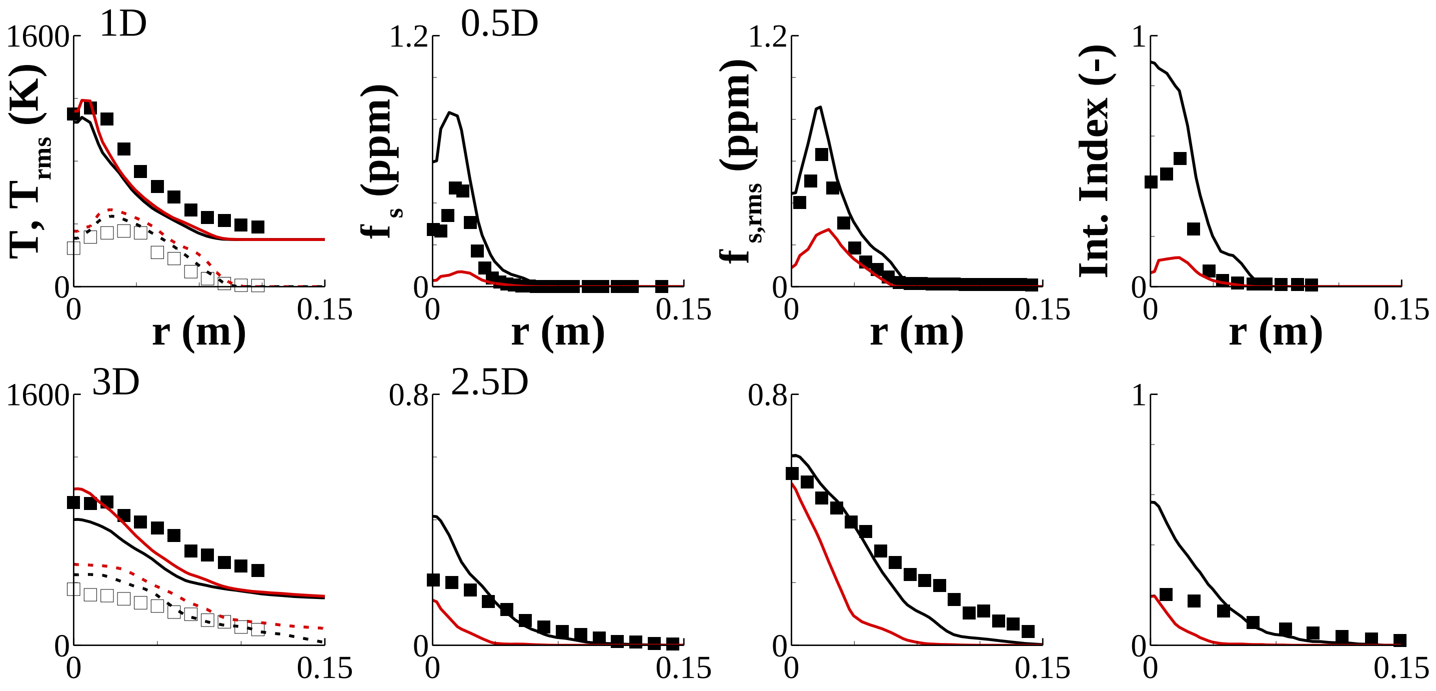
(Xiong et al. 2021)

20.9% 16.8% 15.2%

RESULTS AND DISCUSSIONS

- Comparison with experimental data
  - Experimental observations
    - $f_{s,rms} > f_s$
    - Intermittent Index : fraction of time when soot is present with threshold of 0.09 ppm
      Int. Index < 0.6

Name	Bimodal distribution	« Fast » oxidation
M_1	Yes	Yes
M_2	Yes	No



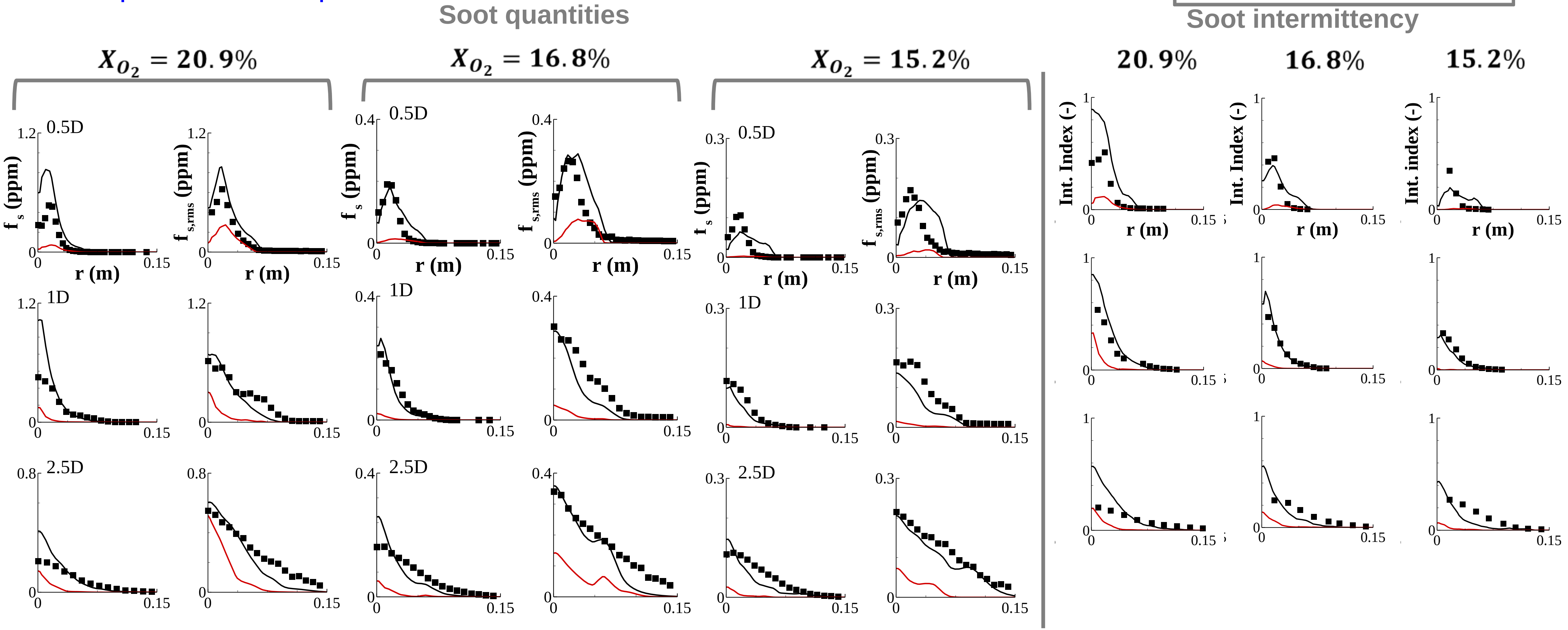
- M_2 : neglecting the (f_s, Z)-correlation creates a chain effect
  1. Overestimated oxidation rate
  2. Underestimated soot quantities
  3. Reduction of soot radiation contribution
  4. Temperature rises especially at the vicinity of the flame axis

- M_1 : Reasonable agreement with exp. data improves significantly the predictions vs M_2

RESULTS AND DISCUSSIONS

- Comparison with experimental data

M_1 : Baseline model
M_2 : (f_s, Z)-correlation neglected



- M_1 in agreement with exp. data for all X_{O_2}
- Global soot ↘ is captured
- Importance of the (f_s, Z)-correlation

RESULTS AND DISCUSSIONS

- Comparison with experimental data: radiative properties

With baseline model M_1

X_{O_2}	χ_R(exp)	χ_R	$\frac{\dot{Q}_{em,s}}{\dot{Q}_{em}}$	$\frac{\dot{Q}_{abs}}{\dot{Q}_{em}}$
20.9%	0.340	**0.389**	**0.496**	**0.261**
16.8%	0.300	**0.255**	**0.370**	**0.286**
15.2%	0.222	**0.192**	**0.267**	**0.322**

Radiant fraction

- χ_R decreases with X_{O_2} owing to conjugated effect of :
  - Temperature decrease
  - Soot reduction
- χ_R within about 15% of the experiment

Soot emission

- For $X_{O_2} = 20.9\%$: $\dot{Q}_{em,s} \approx \dot{Q}_{em,g}$
- For $X_{O_2} = 15.2\%$: $\dot{Q}_{em,s}$ ↘ down to 26.7% of total emission

Flame optical thickness

- The flame becomes optically thicker as the ratio increases with O_2 reduction from 26.1% to 32.2%
- Radiatively participating gases have a stronger non-grey behavior than soot particles

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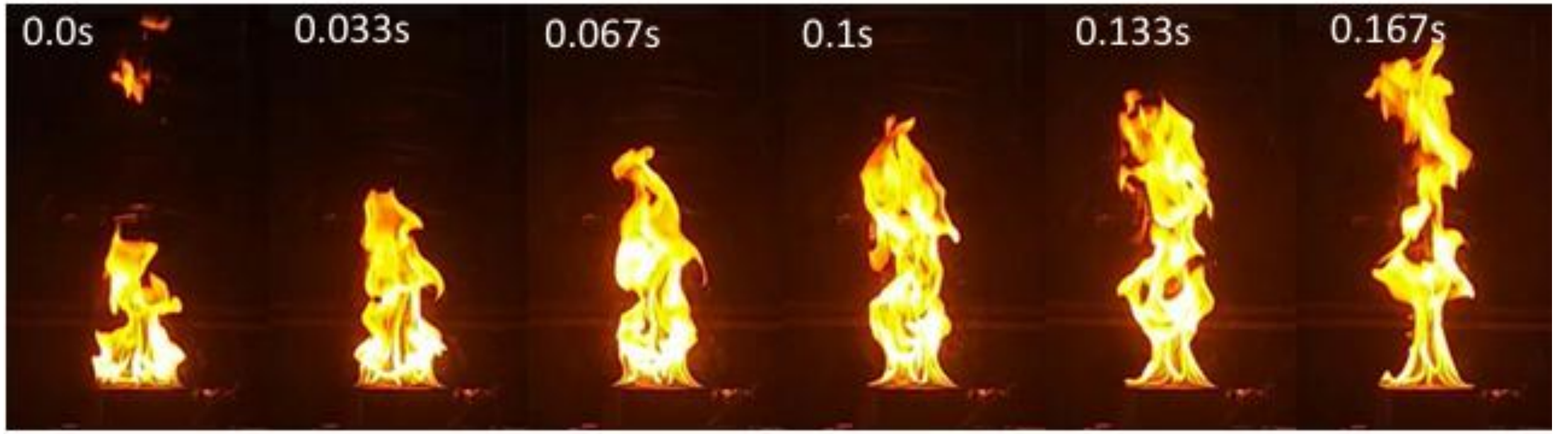
RESULTS AND DISCUSSIONS

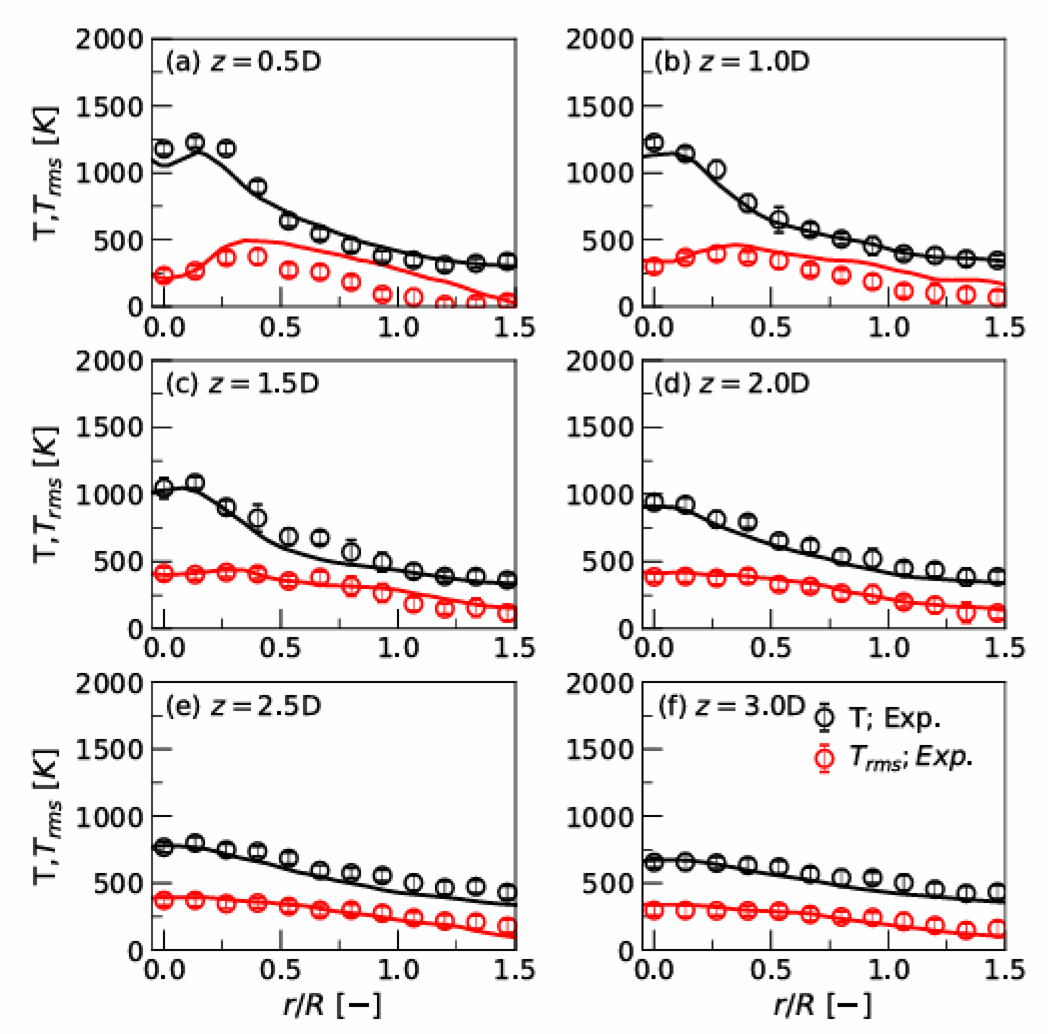
- **15 cm heptane pool fire (Mazurek et al., 2023 - EDF)**
  - HRR: 8.82 kW (χ_a=0.93)
  - Mean SVF: Laser Extinction at 632 nm
  - Temperature: Dual thermocouple technique
  - Radiative loss and radiant fraction: infinite cylinder
  - Total heat feedback to the fuel surface (Kim et al., 2019)

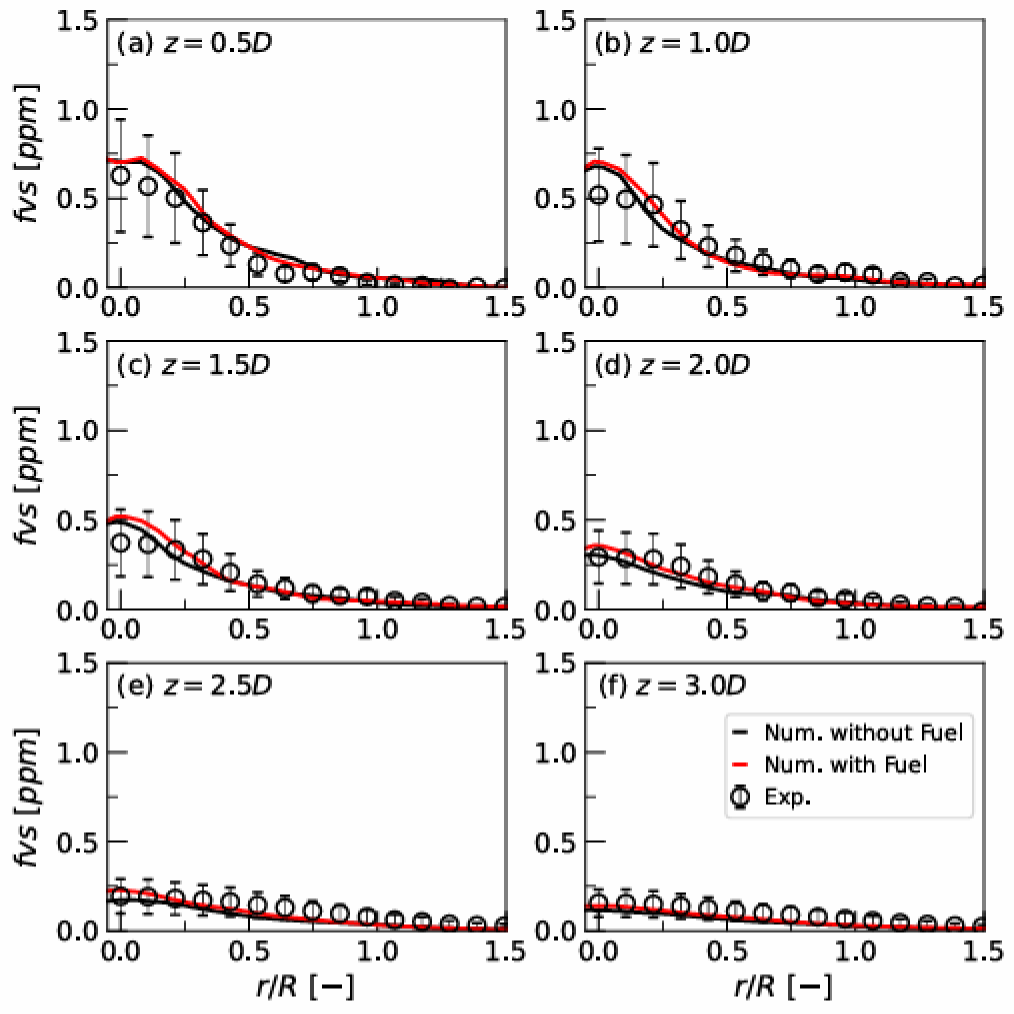
- Computational details
  - M1 is considered
  - Simulation time 50s, Δt =0.5ms
  - Domain: 3×3×1.5 m^3 with minimal size cell of 2.5 mm
  - With and without considering heptane radiation



RESULTS AND DISCUSSIONS

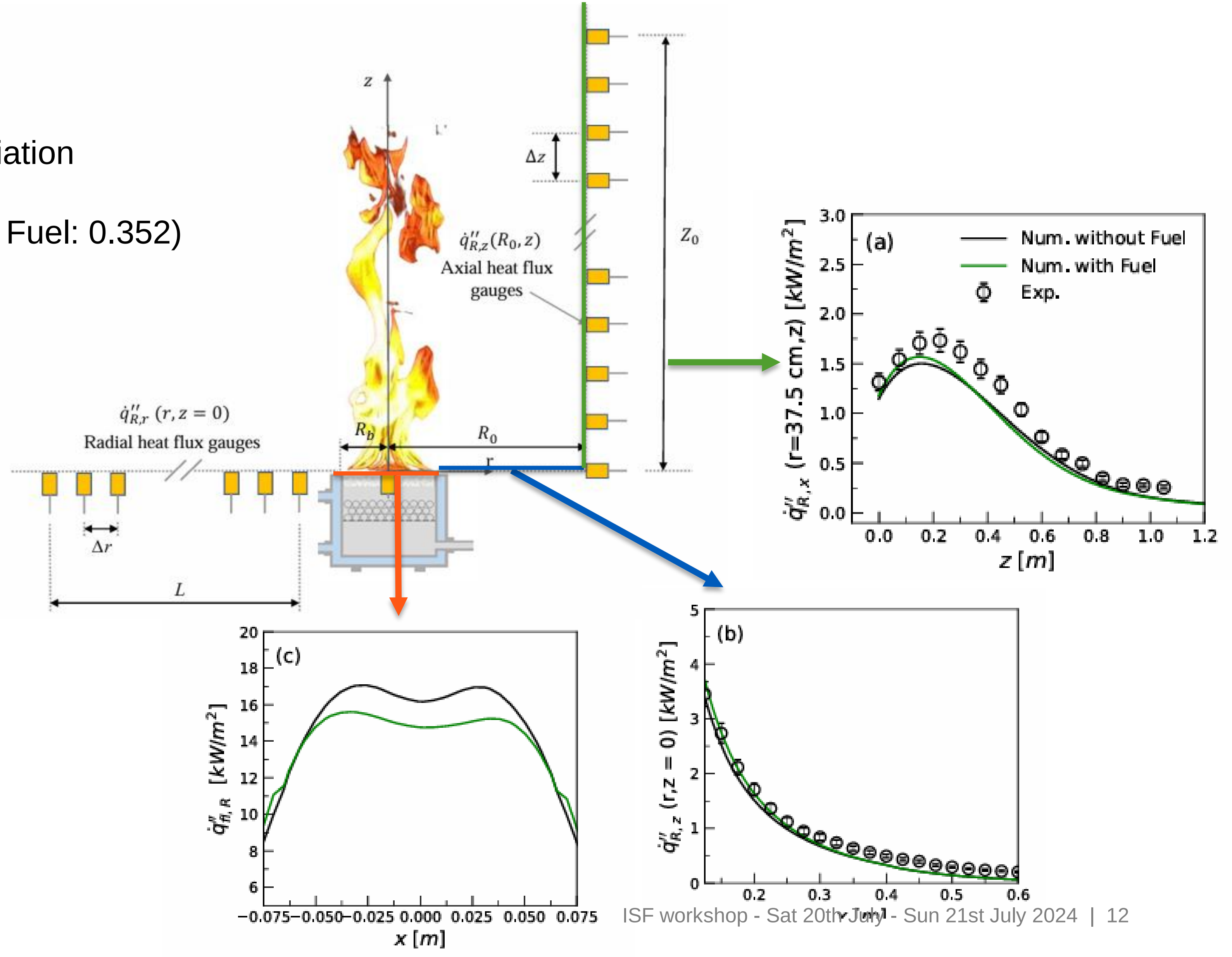
- Flame structure





RESULTS AND DISCUSSIONS

- Radiative and heat feedback outputs
  - Vertical and radial distributions
    - ✓ Good agreement
    - ✓ Not significantly affected by heptane radiation
  - Rad. Fraction (Exp.: 0.37±0,065, Mod. with Fuel: 0.352)
  - Radiative feedback
    - ✓ Heptane radiation: clear impact
    - ✓ Neglecting fuel radiation overestimates the rad. feedback by 10%.



RESULTS AND DISCUSSIONS

Model	$\dot{Q}_{em}$ (kW)	$\dot{Q}_{abs}$ (kW)	$\dot{Q}_{em,s}$ (kW)	$\frac{\dot{Q}_{em,s}}{\dot{Q}_{em}}$ (-)	$\frac{\dot{Q}_{abs}}{\dot{Q}_{em}}$ (-)	χ_R (-)	$\dot{q}''_{fl}$ (kW/m^2)
with Fuel	4.49	1.36	1.80	0.401	0.303	0.352	19.02
without Fuel	4.22	1.22	1.78	0.422	0.289	0.337	20.53
Relative error in %							
	-6.01	-10.3	-1.11	5.22	-4.55	- 4.15	7.94

- Soot emission: 40%
- Radiative gas emission: 60%

- Optical thickness
- 30% emission is reabsorbed within the flame

- Total heat feedback to the center of the fuel surface
- Exp. 18.5 kW/m^2 vs. Model with Fuel 19.02 kW/m^2
- without Fuel: overestimation by about 8%

CONCLUSIONS

- LES of ethylene and heptane pool fires by using a 2 Eqs. C_2H_2/C_6H_6-based soot model and a detailed modeling of gas/soot radiation.

- Account for the correlation between mixture fraction and oxidative species (mixture fraction) to close accurately the filtered soot oxidation rate

- LES reproduces reasonably well the sooting flame structure as well as the radiative loss to the surroundings.

- The radiative contribution of heptane vapor reduces the radiative heat feedback by more than 10 %.