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A three-equation model for the prediction of soot emissions in LES of gas turbines

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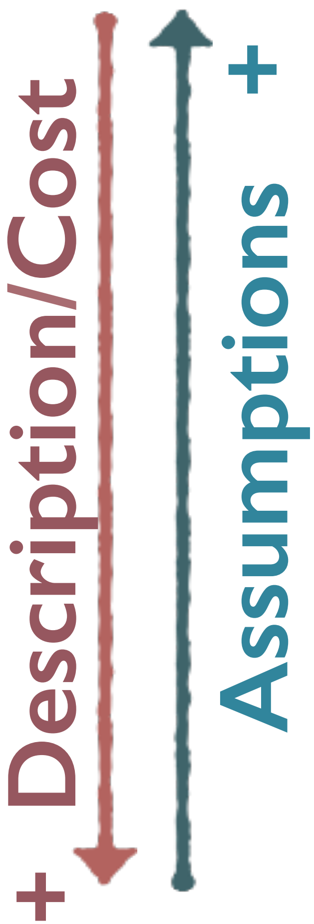
Context – Eulerian soot modeling

Design of low-emission burners = LES param. studies of real configurations

➔ **Development of soot models:**

- Accounting for poly-disperse population of particles
- Minimal CPU cost



Semi-empirical models (2eqns)

+ Access to global quantities
- No access to PSD functions
- Empirical relations for soot source terms

Method of moments (~5eqns)

+ Detailed description of soot production process
- Presumed PSDF shape
- Closure models and numerical issues

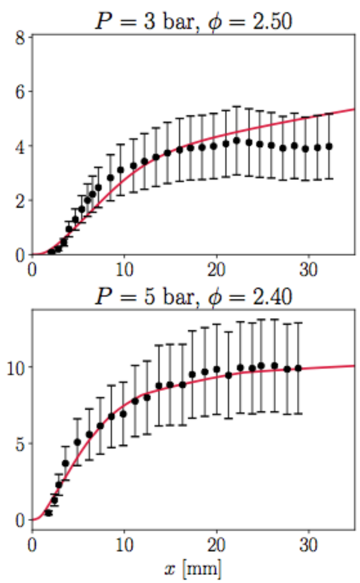
Sectional models (~25eqns)

+ Detailed description of soot production process
+ Low assumptions on PSDF shape
+ Converges towards a continous description
- CPU cost

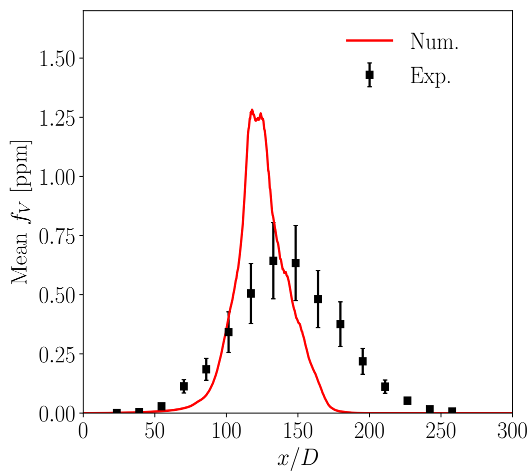
M.E. Mueller and H. Pitsch, *Physics Fluids (2013);* G. Lecocq et al., *Flow, Turb., Combust. (2014);* M. Grader et al., *ASME Turbo Expo* (2018); H. Koo et al., *AIAA (2015);* P. Rodrigues et al. *Comb. Flame (2018).*

State-of-art on LES of sooting turbulent flames

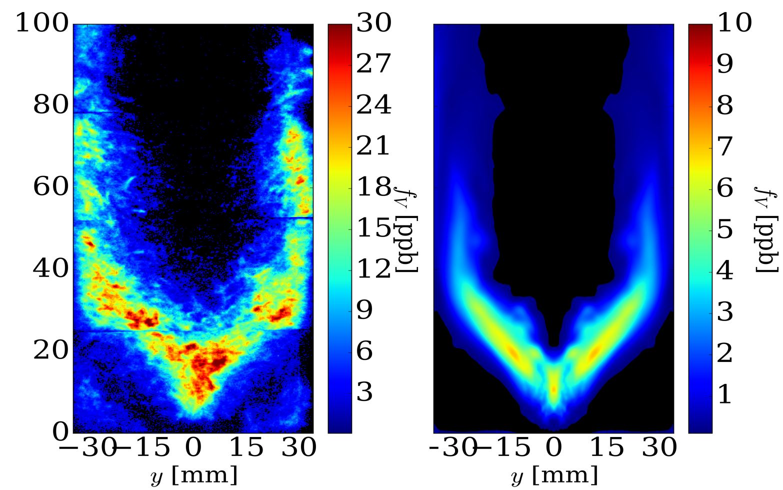
A sectional method for soot has been developed and validated on numerous flames[1]



Laminar premixed flames (P=1,3,5 bar)



Turbulent jet flame



Turbulent swirled flame

Gas phase: 10eqns (NS + look-up table)

Solid phase: 30eqns (PAHs+subgrid+sections)

➔ **High CPU cost: no parametric/industrial studies**

OBJECTIVE

Development of a reliable but cheap model:

- Reduced model *(simpler formulation, physical understanding and implementation)*
- Post-processing PSD reconstruction

[1] P. Rodrigues et al., *Proc. Comb. Inst.* (2017); P. Rodrigues et al., *Comb. Flame* (2018).

Three-equation model

NDF *Bi-variate number density function*

$$f(t, x, v, s)$$

$$\langle \Phi \rangle = \int \int \Phi \mathrm{d}v \mathrm{d}s$$

Global quantities

$N_s = \langle f \rangle$ *Total number density*

$f_v = \langle v f \rangle$ *Soot volume fraction*

$S_s = \langle s f \rangle$ *Total soot surface*

Soot mass fraction $Y_s = \rho_s \rho^{-1} f_v$

Mean particle volume and surface $v_s = f_v N_s^{-1}$ $s_s = S_s N_s^{-1}$

Transport equation

$$\frac{\partial \Psi}{\partial t} + \nabla \cdot (\mathbf{u} \Psi) = \nabla \cdot \left(C_{th} \nu \frac{\nabla T}{T} \Psi \right) + \dot{\omega}_\Psi$$

The source terms are not fitted but derived from the sectional formulation ➔ **NOT** a semi-empirical model!

Closure of source terms

The source terms are not fitted but derived from the sectional formulation by **assuming a mono-disperse distribution**

$$f(v,s) = N_s \delta_{v_s} \delta_{s_s}$$

CONDENSATION

$$\frac{\dot{\omega}_{Y_s}}{\rho_s} = v_{\mathrm{dim}} \beta^{\mathrm{fm}}_{v_{\mathrm{dim}}} N^2_{\mathrm{dim}} + v_{\mathrm{dim}} \beta^{\mathrm{fm}}_{v_{\mathrm{dim}},v_s} N_{\mathrm{dim}} N_s + v_{\mathrm{C_2}} \lambda (k_{\mathrm{sg}} - k_{\mathrm{ox}}) s_s N_s$$

COAGULATION

NUCLEATION

$$\dot{\omega}_{N_s} = \frac{\beta^{\mathrm{fm}}_{v_{\mathrm{dim}}} N^2_{\mathrm{dim}}}{2} - (1 - \mathcal{H}[v_s - v_{\mathrm{C_2}}]) \lambda k_{\mathrm{ox}} s_s N_s - \frac{\beta_{v_s} N_s^2}{2}$$

$$\dot{\omega}_{S_s} = (18\pi)^{1/3} (v_{\mathrm{dim}})^{2/3} \beta^{\mathrm{fm}}_{v_{\mathrm{dim}}} N^2_{\mathrm{dim}} + \delta s^{\mathrm{frac}}_{v_{\mathrm{dim}}} \beta^{\mathrm{fm}}_{v_{\mathrm{dim}},v_s} N_{\mathrm{dim}} N_s + \lambda (\delta s^{\mathrm{frac}}_{v_{\mathrm{C_2}}} k_{\mathrm{sg}} - \delta s^{\mathrm{spher}}_{v_{\mathrm{C_2}}} k_{\mathrm{ox}}) s_s N_s$$

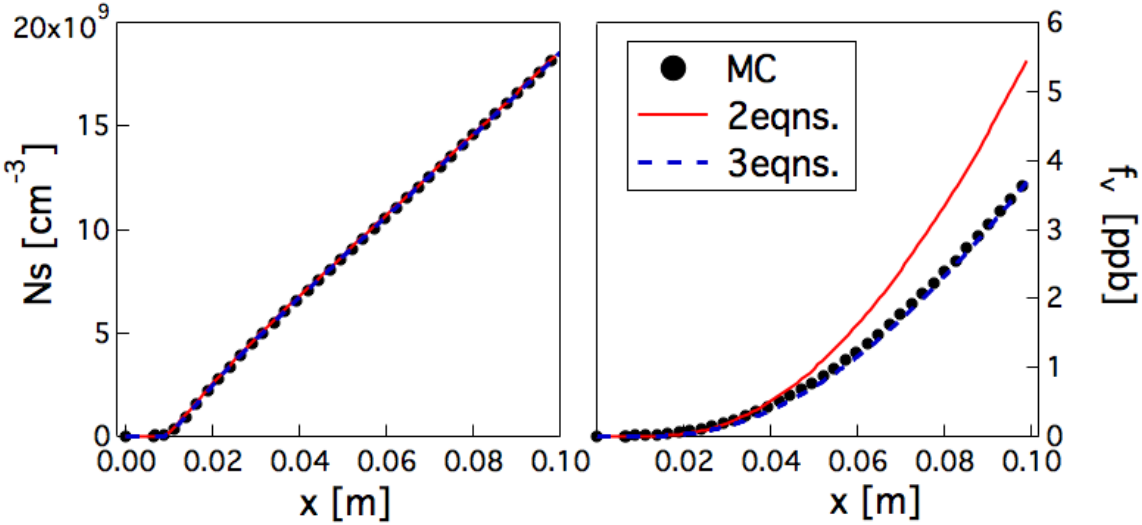
Validation for global quantities: premixed flame

Comparing with reference description (Monte-Carlo)

CoMo GROUP

Monte-Carlo Sweep code[1]

NUCLEATION & SURF. GROWTH

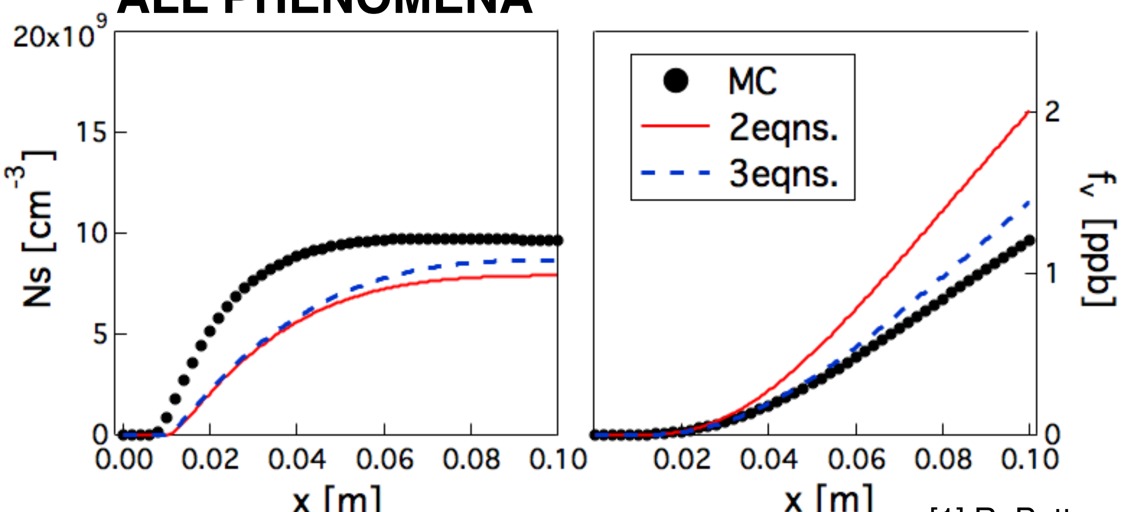


$$s_s^{2\mathrm{eq}} = (36\pi)^{1/3} v_s^{2/3}$$

$$s_s^{3\mathrm{eq}} = S_s N_s^{-1}$$

Equation for surface improves the accuracy

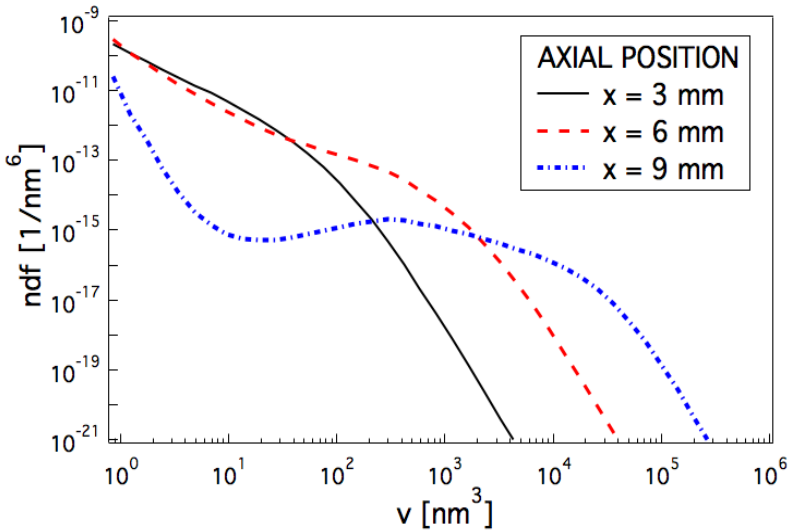
ALL PHENOMENA



- Reasonable description with 3-eqns
- Discrepancies are found for bimodal distributions

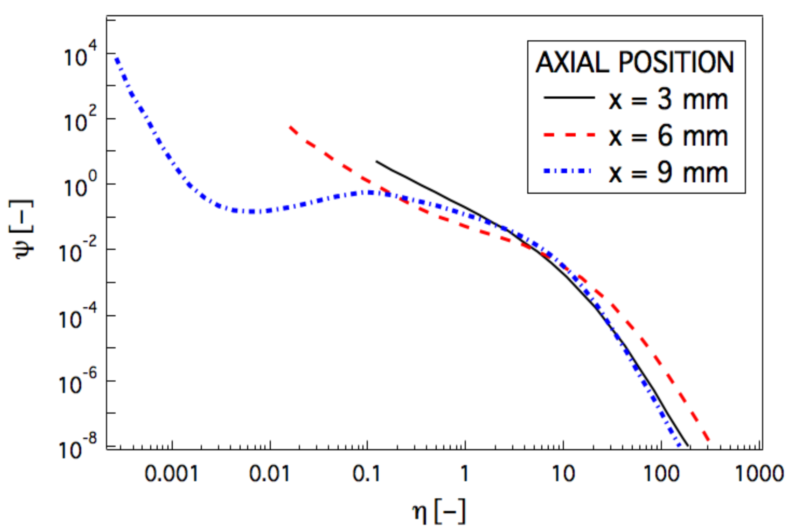
[1] R. Patterson et al. *J. SIAM on Scientific Computing* (2006).

Marginal NDF



$$n(v) = \int f(v, s)\mathrm{d}s$$

Results for a laminar premixed flame[1] using a sectional method[2]



DIMENSIONLESS NDF

$$\psi(\eta) = n f_v / N_s^2$$

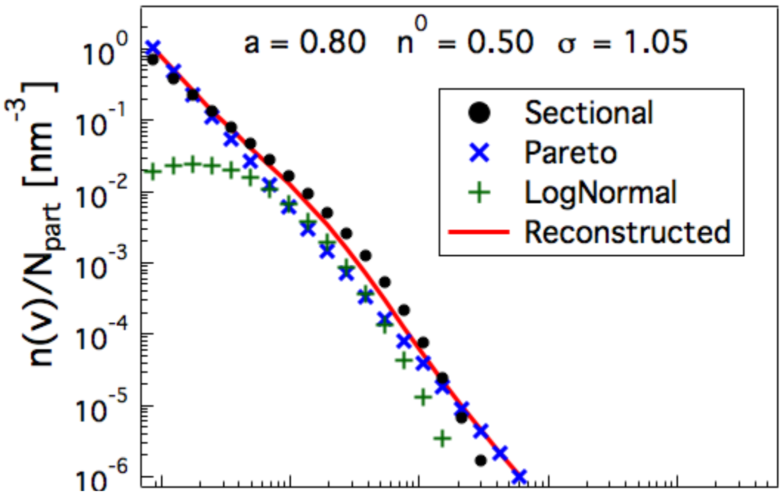
$$\eta = v / v_s$$

Self-similarity[3] does not apply to soot NDF

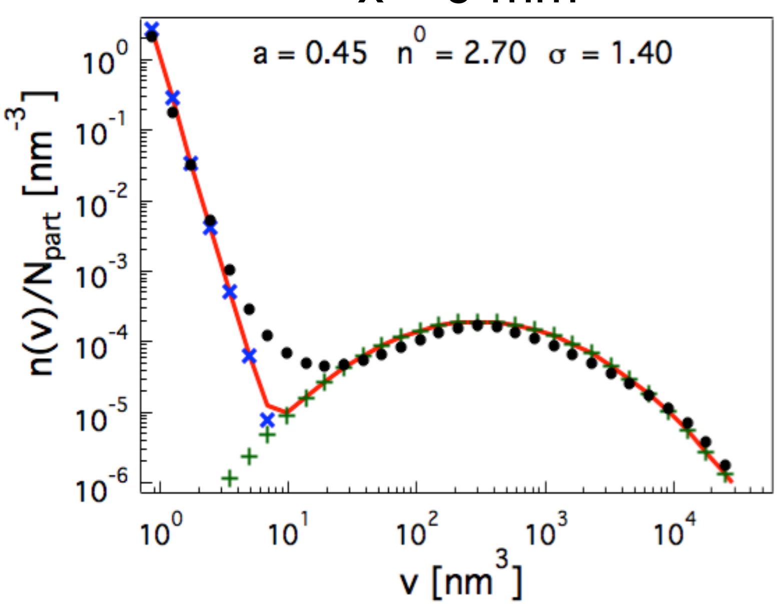
[1] A.D. Abid et al., *Comb. Flame* (2008).
[2] P. Rodrigues et al. *Proc. Comb. Inst.* (2017).
[3] F. Jun et al. *Fire Sci.* (2004).

Reconstruction of the NDF

x = 3 mm



x = 9 mm



Reconstructed NDF (R-NDF)

$$\bar{n}(v) = \frac{n(v)}{N_s} \approx a\bar{\mathrm{n}}_1(v) + (1-a)\bar{\mathrm{n}}_2(v)$$

Pareto **LogNormal**

Distributions parameters are analytically derived except for:

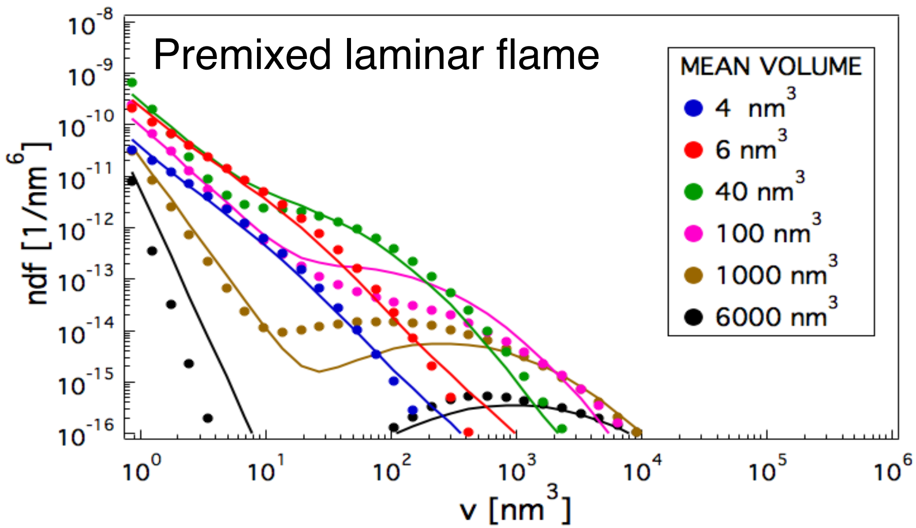
$$a = \max\left[0, 1.0 - 0.18\left(\frac{v_s}{v_{\mathrm{nucl}}}\right)^{0.12}\right]$$

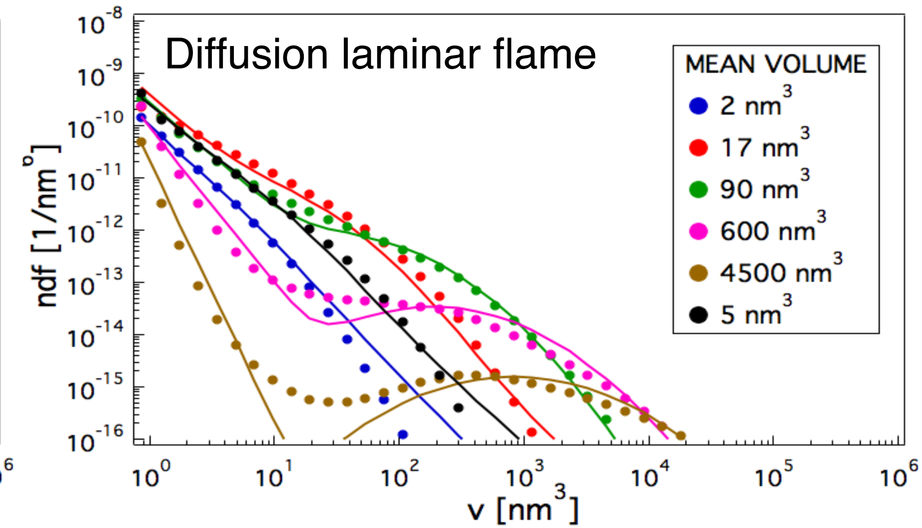
$$\bar{\mathrm{n}}^0 = 8(1-a)^2 \quad \sigma = 1 + 0.65(1-a)$$

v_s determines the R-NDF shape:

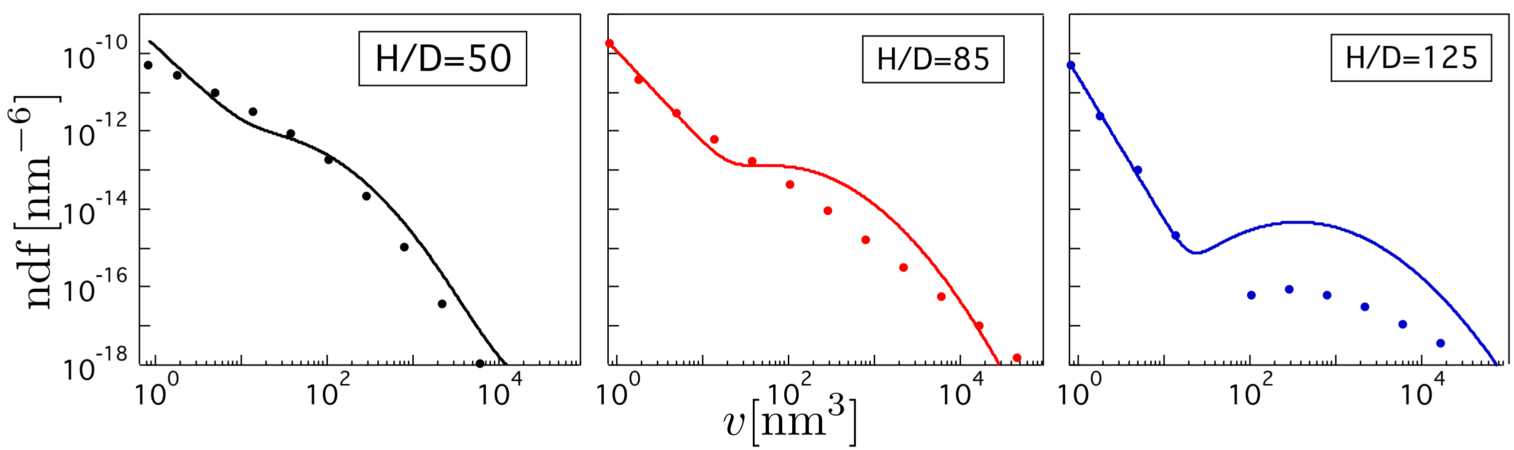
- Small v_s (f_v): one-peak
  ➔ Pareto
- Large v_s (f_v): two-peaks
  ➔ Pareto+Lognormal

A priori R-NDF validation: sec (sym) vs 3eqns (line)





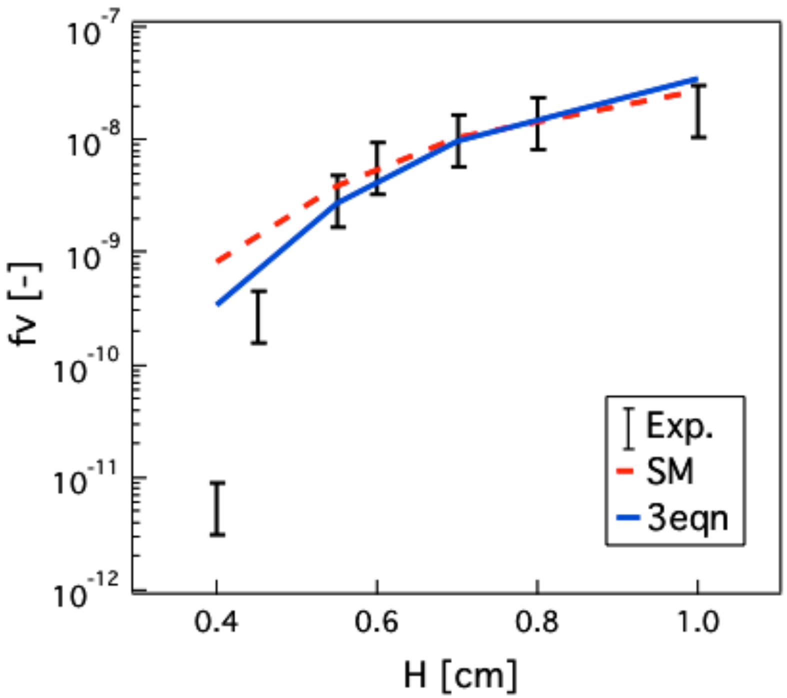
Turbulent jet flame (instantaneous results)

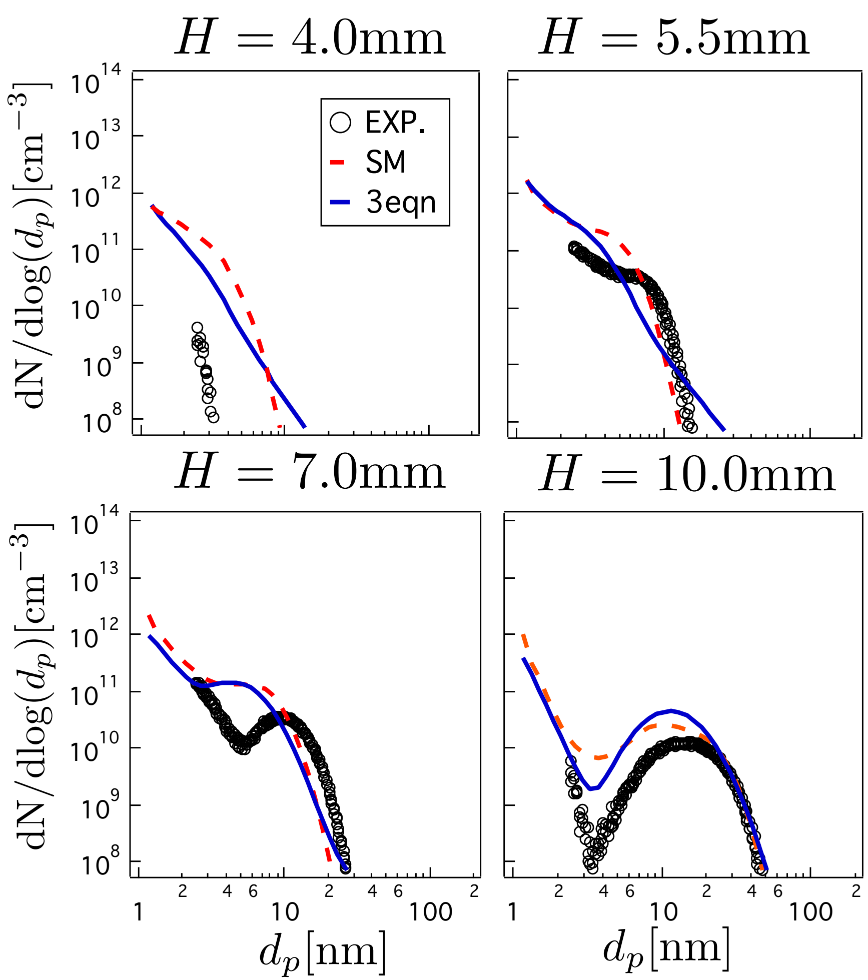


- R-NDF correctly reproduces the ndf-shape (one-/two-peaks).
- Empirical R-NDF relations ➔ dependence on fuel/operating conditions BUT decomposition into Pareto and logNormal seems general.

A posteriori validation: laminar-ISF benchmark

Burner Stabilized Stagnation laminar premixed oxygen/argon/ethylene flame[1,2]





- Good agreement with SM and experiments.
- Accuracy is representative of the state-of-art soot modeling.

[1] C. Saggese et al. *Comb. Flame* (2015).
[2] P. Rodrigues et al. *Proc. Comb. Inst.* (2017).

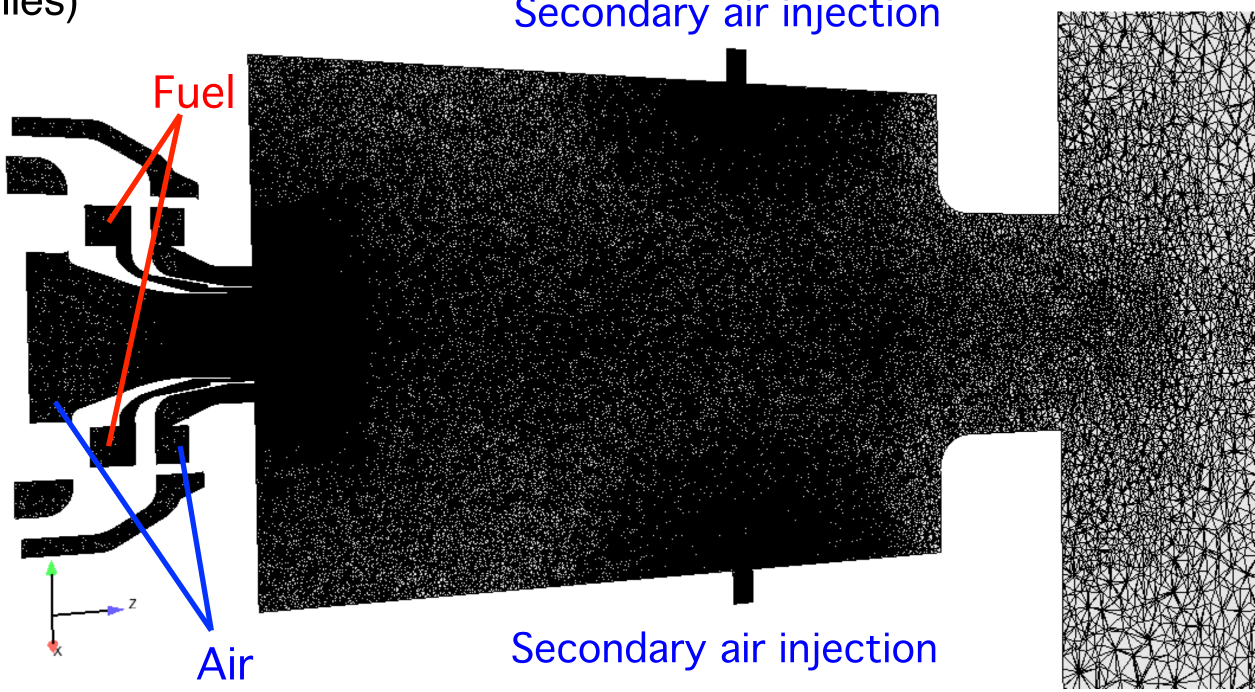
A posteriori validation: DLR[1]-ISF benchmark

Solver: AVBP

(CERFACS/IFP Energies nouvelles)

Setup already validated for SM

- *Gas phase: RFPV model from KM2 mechanism + beta-pdf*
- *Solid phase: intermittency model*
- *Radiation: optically-thin model*
- *Experimental temperature imposed on chamber wall*



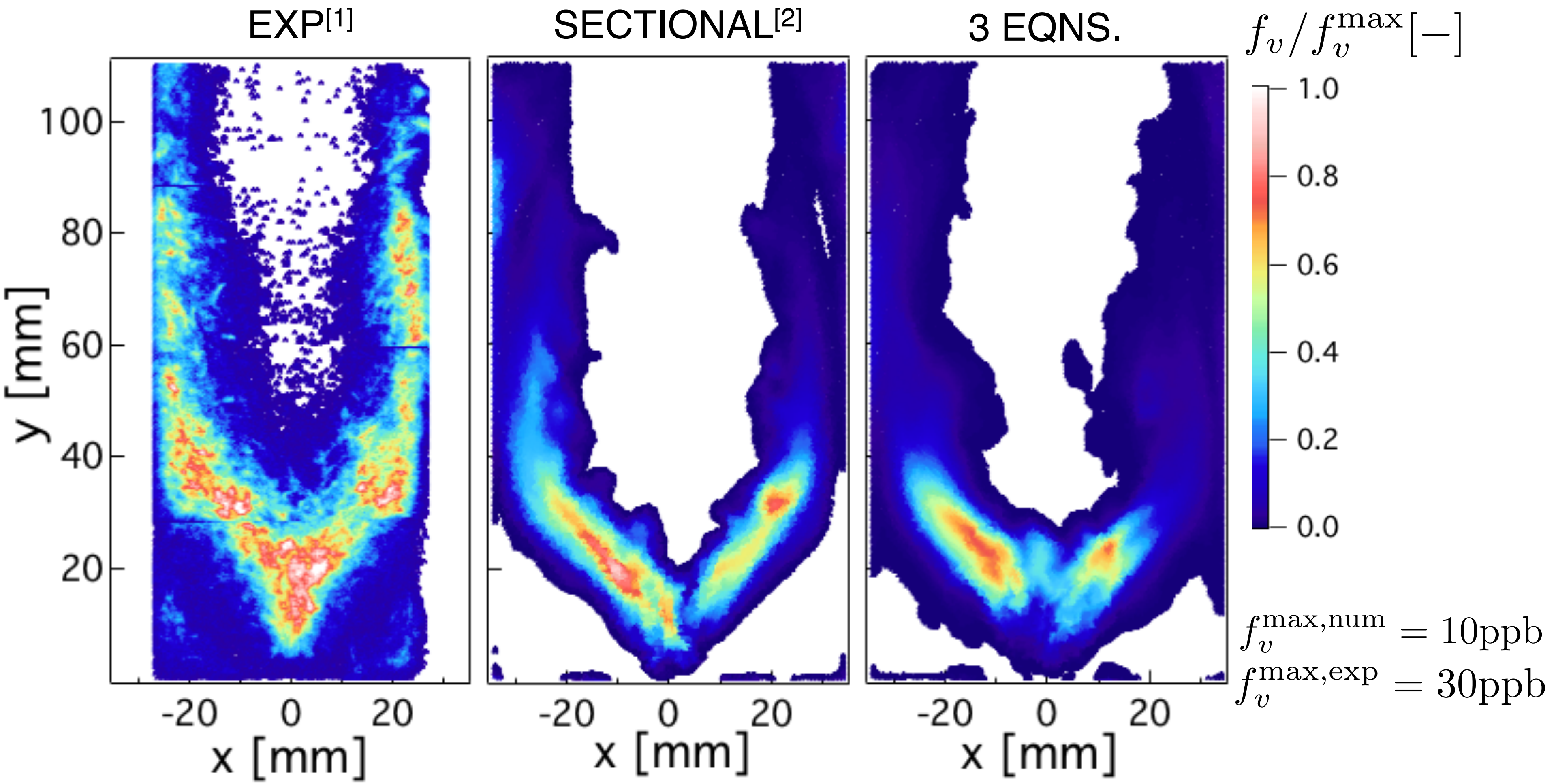
Operating point

T=300 K
P=3 bar
Q_{oxi}/Q_{air}=0.4

Scheme	TTGC: 3rd order in time and space
Cells	40,000,000
SGS model	WALE
Av. time	30ms

[1] K.P. Geigle et al. *ASME Turbo Expo* (2011).

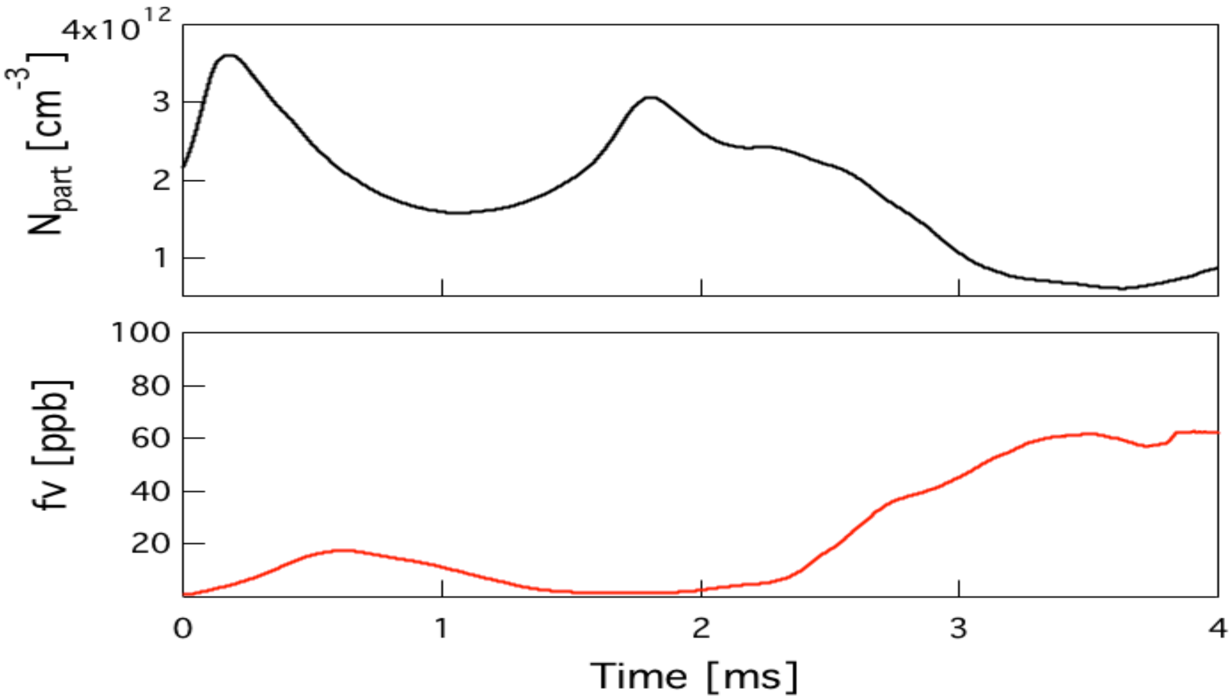
LES results on FIRST test rig

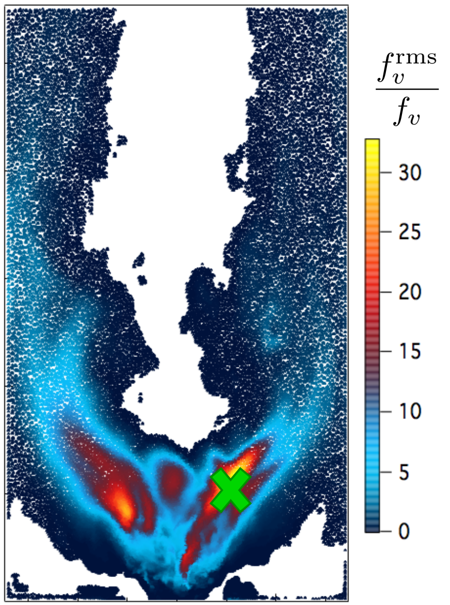


- Good agreement with experiments (soot yield and position)
- Satisfactory agreement sectional VS 3eqns (and CPU cost reduced by 3!)

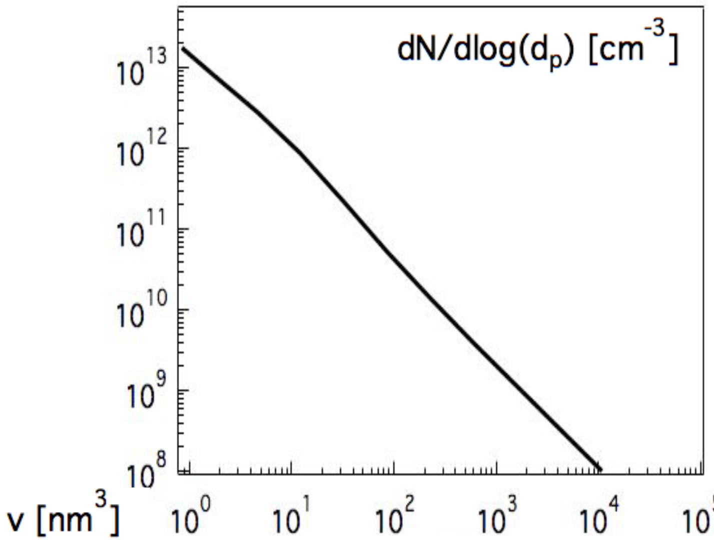
[1] K.P. Geigle et al. *ASME Turbo Expo* (2011).
[2] P. Rodrigues et al. *INCA* (2017).

High fluctuations of soot quantities

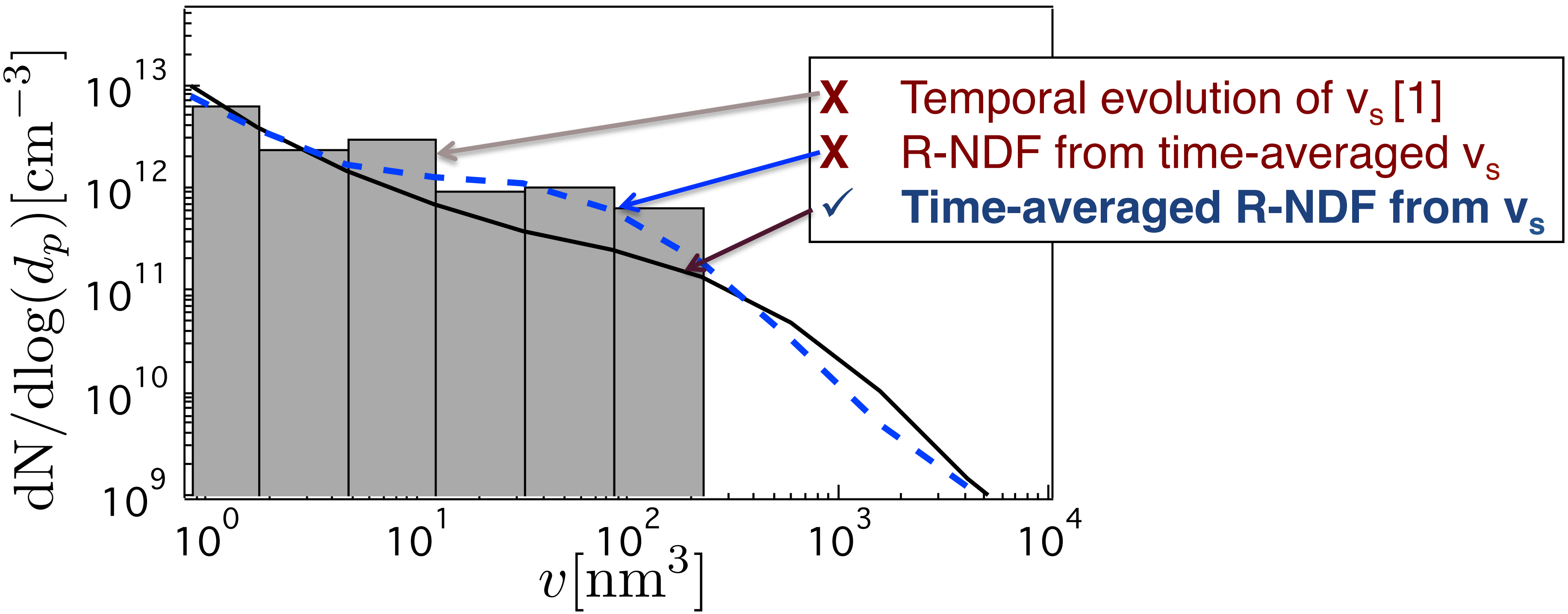




- PSD strongly varies in space and time
- Time-averaged PSD is almost everywhere one-peak (as for sectional)



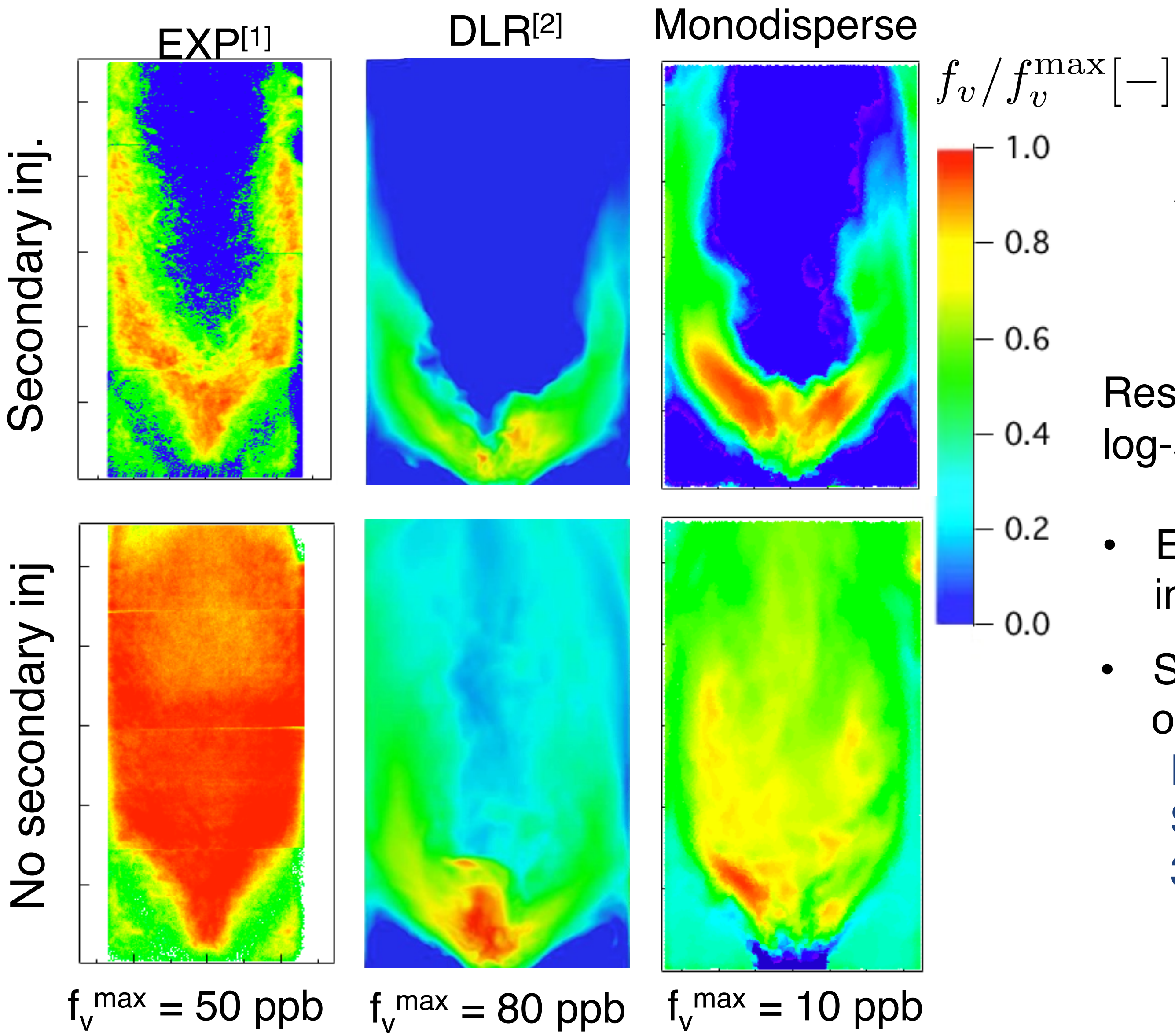
Have to obtain time-averaged PSD?



High non-linearity of PSD with respect to moments: the temporal evolution of the PSD (reconstructed or transported) has to be averaged during the computation

N.B. No PSD validation is provided by comparison with experimental data (not available for this configuration)

Secondary air injection effect



DLR: detailed chemistry + SM for PAH and soot

Results are represented in log-scale!!!

- Effect of secondary air injection is captured
- Similar results than state-of-art but smaller CPU cost

  DLR ~ 70 eqns
  SM ~ 40 eqns
  3EQNS ~ 15 eqns

[1] K.P. Geigle et al. *ASME Turbo Expo* (2013)

[2] M. Grader et al., *ASME Turbo Expo* (2018)

Conclusion

Development of a reliable soot model for LES of gas turbine:

1. *New equation for total soot surface: better description of surface reactions*
2. *Theoretical development: larger validity compared to empirical models*
3. *Easy implementation into CFD solver*
4. *Reasonable estimation of the PSD*
5. *Low CPU cost*

- R-NDF requires more validation
- 3eqns accuracy is reduced when NDF is highly poly-disperse.

STILL →

Good candidate for LES of gas turbines: fv small (< 1ppm) ➔ monodisperse population.

Acknowledgement

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GENCI