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LES/PDF Modeling of Turbulent Reacting Flows

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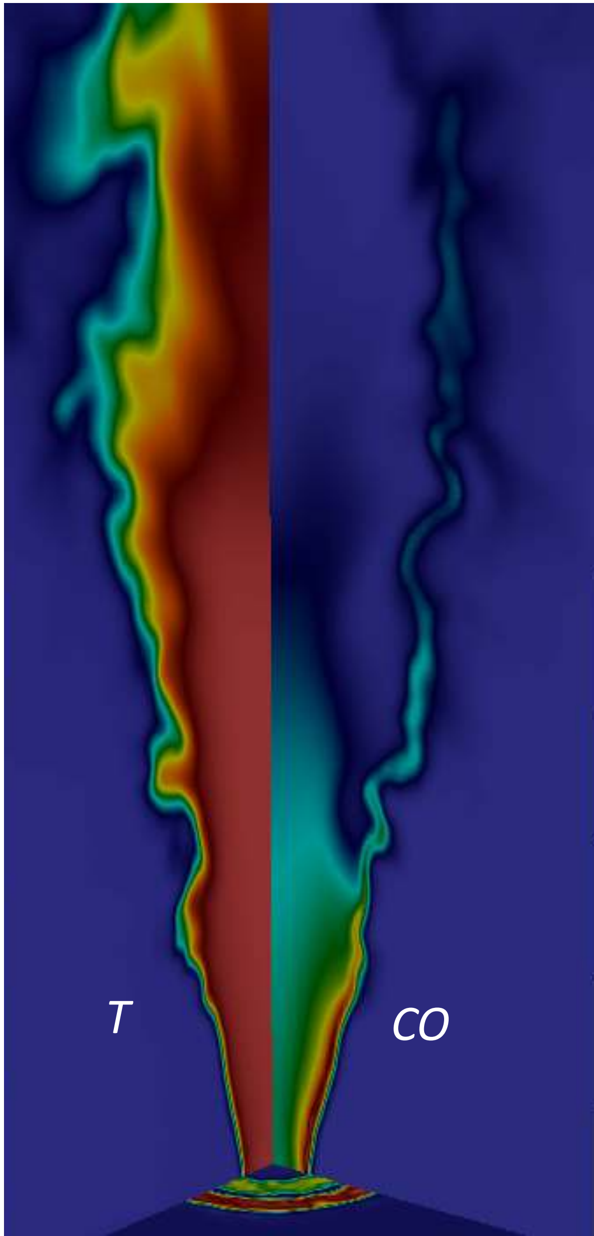

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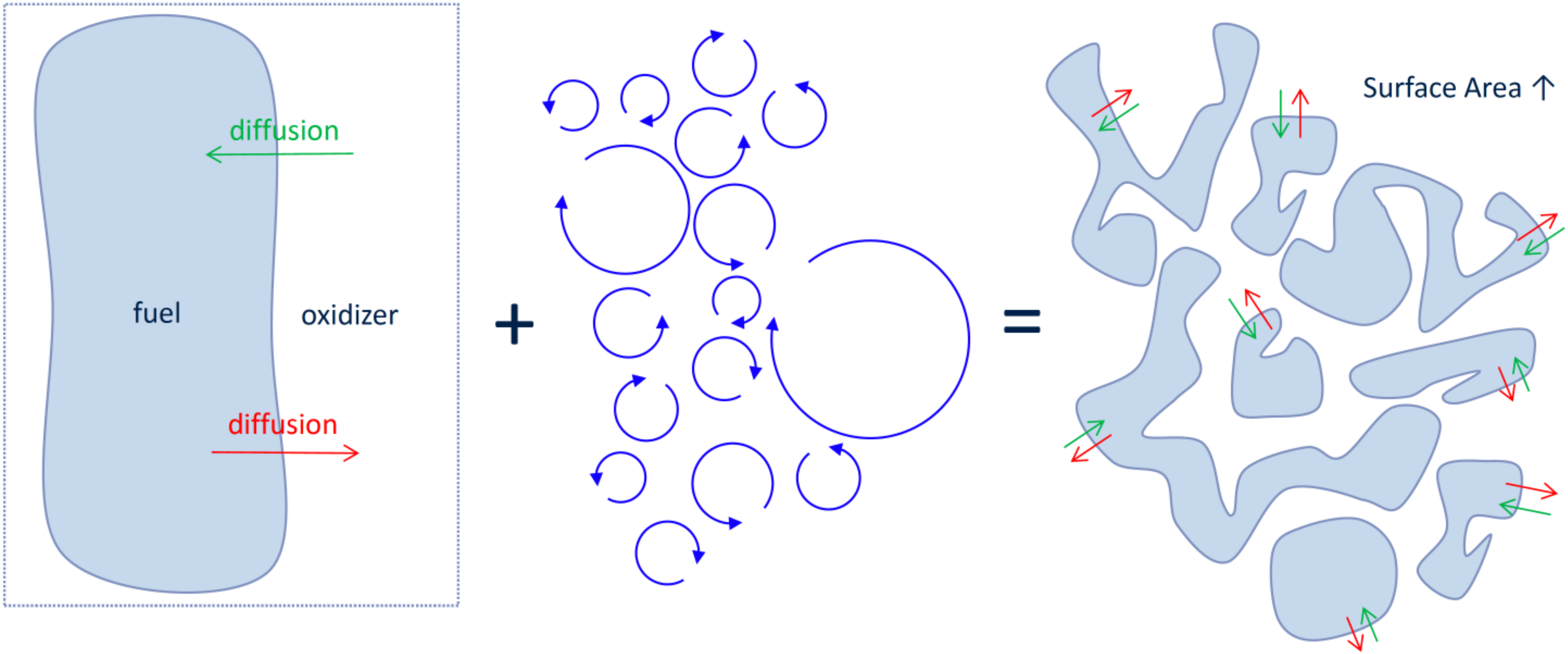
Outline

- Motivations
- LES/PDF Method
- Numerical Solution Algorithm
- Cambridge/Sandia Stratified Flames
  - Non-swirling flames
  - Swirling flames
- Results and Comparison with Experimental Data
- Conclusions

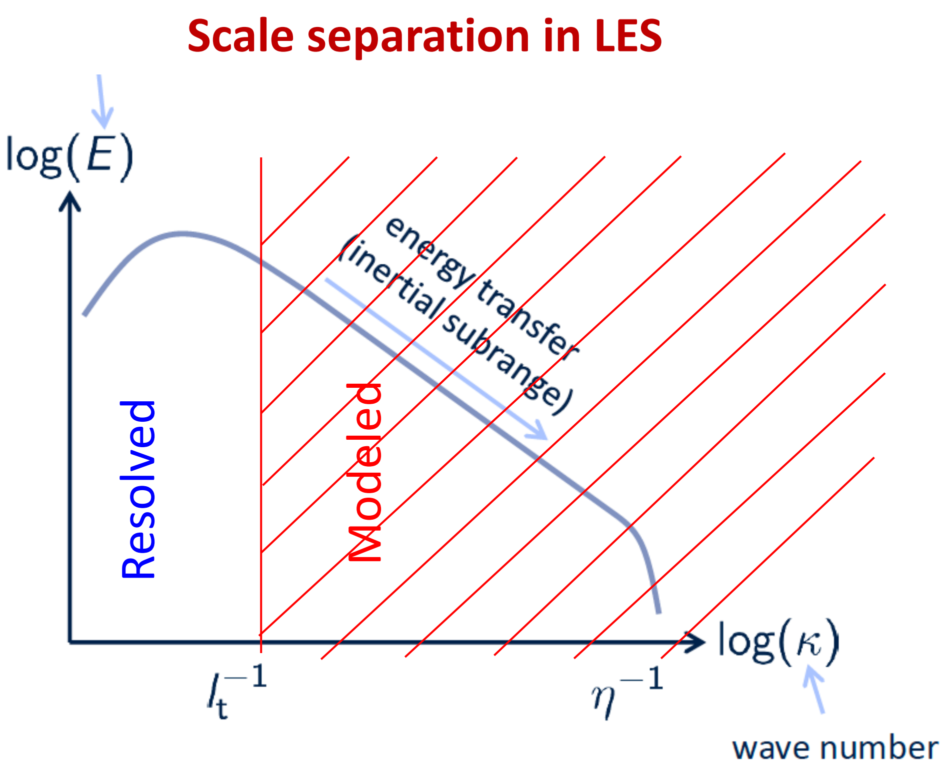
Why turbulent combustion?



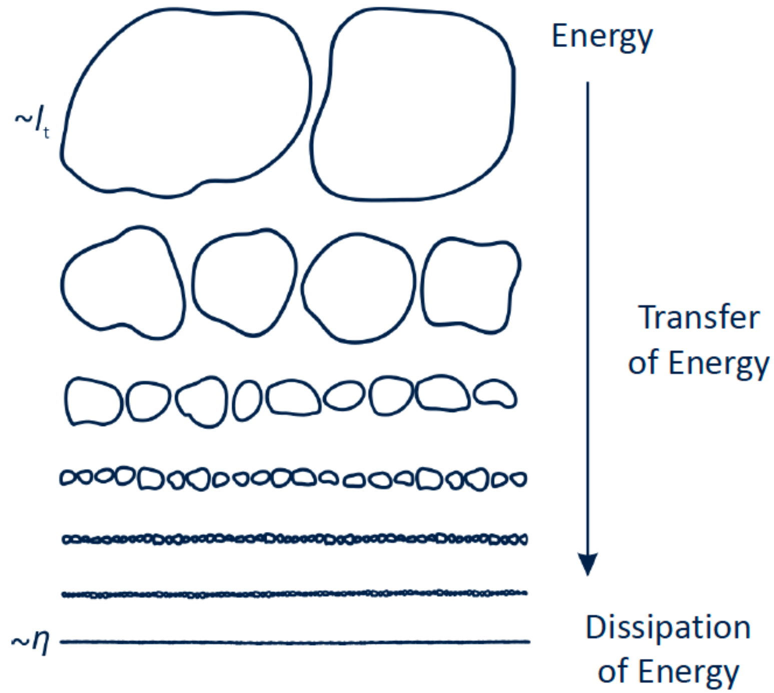
- Combustion requires mixing at the molecular level
- Turbulence: enhanced convective transport + molecular mixing

Why LES?

Energy Spectrum (logarithmic)

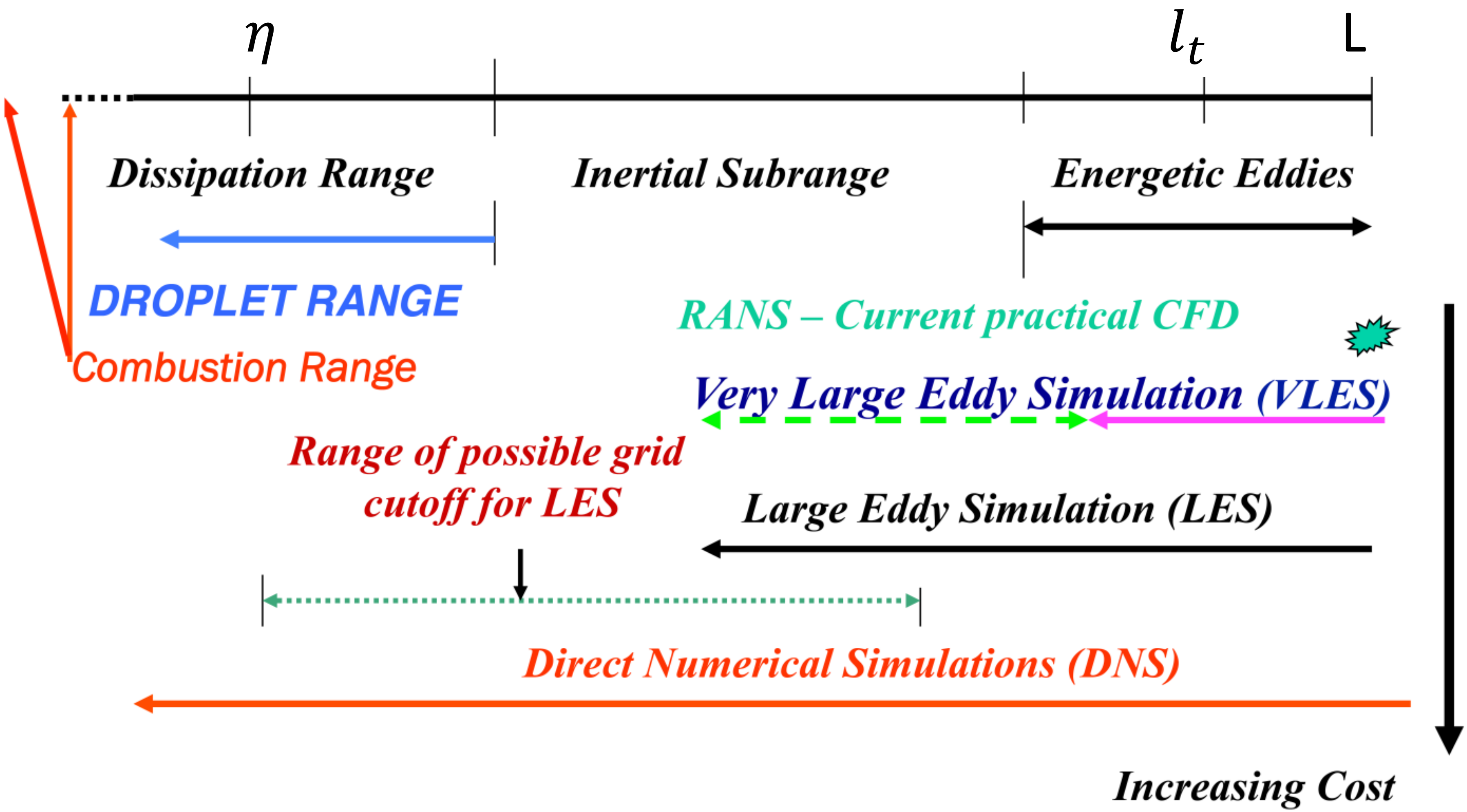


Energy Cascade



- **The energy cascade and Kolmogorov's hypotheses:**
  - Energy is extracted from large scale and cascaded to smaller scales until its dissipation
  - The small scale motion is ``universal"
- **In LES:** Resolve the large scale motion and model the ``universal" small scale motion
  - Modelling is still an issue but it is theoretically possible to develop a flow-independent model

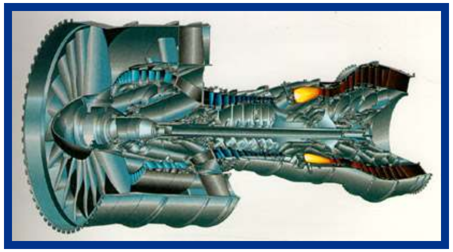
Modeling of Turbulent Reacting Flows

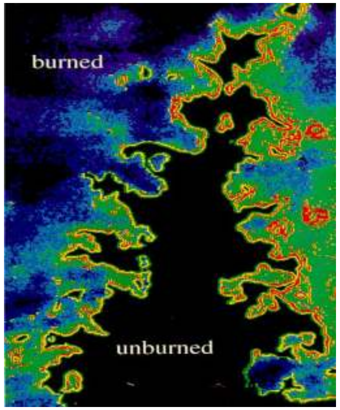


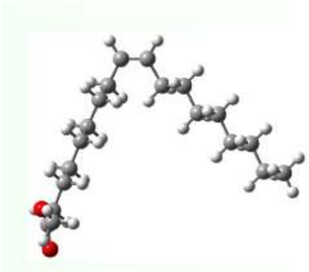
For LES: Resolve at least 80% of turbulent kinetic energy (Pope 2004)

Scale Separation in Combustion?

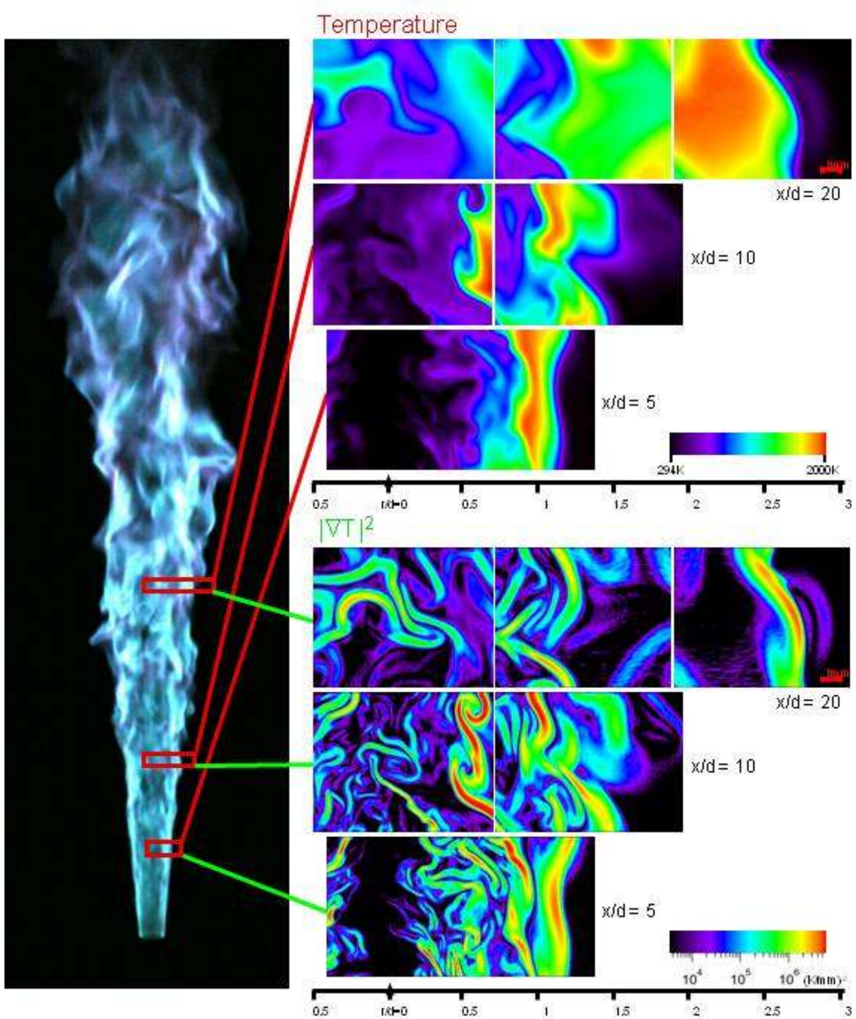
- Typical range of spatial scales
  - Scale of combustor: 10 – 100 cm
  - Energy containing eddies: 1 – 10 cm
  - Small-scale mixing of eddies: 0.1 – 10 mm
  - Diffusive-scales, flame thickness: 10 – 100 μm
  - Molecular interactions, chemical reactions: 1 – 10 nm
- Spatial and temporal dynamics inherently coupled
- All scales are relevant and must be resolved or modeled
- In particular, chemical reactions occur at molecular scale
- So, LES has the same closure problem as RANS







Grand Challenges in Combustion



https://crf.sandia.gov/combustion-research-facility/reacting-flow/flow-experiments/imaging/

- **Stiffness** : wide range of length and time scales
  - combustor (cm)
  - turbulence-chemistry (mm)
  - flame reaction zone (μm)
  - soot inception (nanometer)
- Chemical complexity

  large number of species and reactions (100's of species, thousands of reactions)
- Multi-physics complexity
  - multiphase (liquid spray, gas phase, soot, surface)
  - thermal radiation
  - acoustics ...
- All of these are tightly coupled

S.B. Pope , ``Small scales, many species and the manifold challenges of turbulent combustion", Proc. Combust. Inst., 34(1):1-31 (2013)

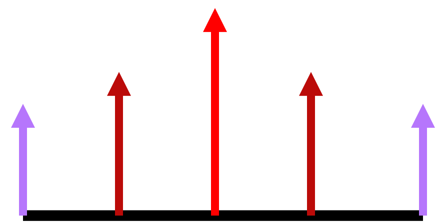
Modes of Combustion

Non-premixed

Oxidizer Fuel

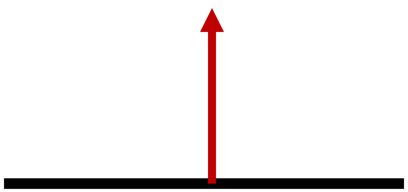
- High NOx, Soot
- Good dynamics range

Stratified



Fuel + Oxidizer at different ϕ

Premixed



Fuel + Oxidizer

- Low NOx, Soot,CO
- Narrow dynamics range

Combustion usually takes place in a stratified mode in gas turbine combustors:

- The limited time and length scales imposed by design constraints that prevent fuel from mixing with oxidizer (unintentional).
- The stratification is created to increase the flame stability for lean combustion (intentional).
- A rich burn/quench/lean burn (RQL) combustion is common in many aero engines (intentional).
- **PDF method is well suited**: No inherent assumption on the type of combustion

Reacting Flows: Mathematical Model

- The mass conservation:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_j}{\partial x_j} = 0$$

- The momentum conservation:

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i; \qquad \tau_{ij} = \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) - \frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}$$

- The energy and species mass conservation (n_s species involved):

$$\frac{\partial \rho \phi_\alpha}{\partial t} + \frac{\partial \rho u_j \phi_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j}\left(\rho D_\alpha \frac{\partial \phi_\alpha}{\partial x_j}\right) \boxed{+\, \rho S_\alpha}$$

$$\boldsymbol{\phi} = \left[\phi_1, \phi_2, \phi_3, \dots, \phi_{n_s}, h\right]$$

- The equation of state:

$$p = \rho R T$$

$S_\alpha = S_\alpha(\boldsymbol{\phi}, x, t)$
Highly non-linear function of mass fractions and temperature (enthalpy)

The Filtering Operation in LES

- The definition of low-pass filter:

$$\bar{\rho}(\boldsymbol{x}) \equiv \int_{-\infty}^{\infty} \rho(\boldsymbol{y}, t)\, G(\boldsymbol{y} - \boldsymbol{x}) d\boldsymbol{y}$$

$$\tilde{Q}(\boldsymbol{x}) \equiv \frac{1}{\bar{\rho}(\boldsymbol{x})} \int_{-\infty}^{\infty} \rho(\boldsymbol{y}, t)\, Q(\boldsymbol{y}, t) G(\boldsymbol{y} - \boldsymbol{x}) d\boldsymbol{y}$$

- The filtered equations and closure problem:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = 0,$$

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_i \tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tilde{\tau}_{ij}}{\partial x_j} + \frac{\partial T_{ij}}{\partial x_j},$$

$$\tilde{\tau}_{ij} \approx \tilde{\mu} \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \mu \frac{\partial \tilde{u}_k}{\partial x_k} \delta_{ij}; \qquad T_{ij} = \bar{\rho} \tilde{u}_i \tilde{u}_j - \bar{\rho} \widetilde{u_i u_j}$$

$$\frac{\partial \bar{\rho} \tilde{\phi}_\alpha}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{\phi}_\alpha}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{\rho} \tilde{D}_\alpha \frac{\partial \tilde{\phi}_\alpha}{\partial x_j} \right) + \frac{\partial T_{\alpha j}}{\partial x_j} + \bar{\rho} \tilde{S}_\alpha; \qquad T_{\alpha j} = \bar{\rho} \tilde{\phi}_\alpha \tilde{u}_j - \bar{\rho} \widetilde{\phi_\alpha u_j}$$

- Observe that

$$\tilde{S}_\alpha \neq S(\tilde{\boldsymbol{\phi}})$$

- **Main task in combustion is to model the source term!**

The LES/PDF Approach

- The filtered mass density function:

$$\mathcal{F}(\boldsymbol{\psi};\boldsymbol{x},t) \equiv \int_{-\infty}^{\infty} \rho(\boldsymbol{y},t)\,\delta\big(\boldsymbol{\psi}-\boldsymbol{\phi}(\boldsymbol{y},t)\big)G(\boldsymbol{y}-\boldsymbol{x})d\boldsymbol{y}$$

- The Favre-filtered PDF:

$$\tilde{f} \equiv \mathcal{F}(\boldsymbol{\psi};\boldsymbol{x},t)/\bar{\rho}; \qquad \tilde{Q}(\boldsymbol{x},t) = \int Q(\boldsymbol{\psi};\boldsymbol{x},t)\,\tilde{f}(\boldsymbol{\psi};\boldsymbol{x},t)\mathrm{d}\boldsymbol{\psi}$$

- The exact transport equation for the joint PDF of compositions:

$$\frac{\partial \bar{\rho}\tilde{f}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{f}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\bar{\rho}\,\left(\widetilde{u_i''|\boldsymbol{\psi}}\right)\tilde{f}\right) = \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}\left(-\overline{\frac{\partial J_i^\alpha}{\partial x_i}|\boldsymbol{\psi}}\right)\right] \boxed{+\frac{\partial}{\partial \psi_\alpha}\left(\bar{\rho}\tilde{f}S_\alpha(\boldsymbol{\psi})\right)}$$

$$J_i^\alpha = -\rho D_\alpha \frac{\partial \phi_\alpha}{\partial x_i}; \qquad u_i'' = u_i - \tilde{u}_i$$

- The chemical source term is in the closed form
- Arbitrarily non-linear chemical reactions are treated exactly in the PDF methods
- This is the main advantage of the PDF methods

Modeling the Unclosed Terms

- The gradient diffusion assumption:

$$(u_i''|\boldsymbol{\psi})\tilde{f} = -\widetilde{D}_T \frac{\partial \tilde{f}}{\partial x_i}$$

- The Favre-filtered PDF:

$$\left(-\overline{\frac{\partial J_i^\alpha}{\partial x_i}}|\boldsymbol{\psi}\right) = \frac{1}{\bar{\rho}} \overline{\frac{\partial}{\partial x_i}\left(\rho D_\alpha \frac{\partial \phi_\alpha}{\partial x_i}\right)|\boldsymbol{\psi}} = -\Omega(\psi_\alpha - \tilde{\phi}_\alpha) + \frac{1}{\bar{\rho}} \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{D}_\alpha \frac{\partial \tilde{\phi}_\alpha}{\partial x_i} - \bar{\rho}\tilde{\phi}_\alpha V_c\right)$$

- The modeled transport equation for the joint PDF of composition:

$$\frac{\partial \bar{\rho}\tilde{f}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{f}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\bar{\rho}\,\widetilde{D}_T \frac{\partial \tilde{f}}{\partial x_i}\right)$$
$$= \frac{\partial}{\partial \psi_\alpha}[\bar{\rho}\,\tilde{f}\Omega(\psi_\alpha - \tilde{\phi}_\alpha)] - \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}\,\frac{\partial}{\partial x_i}(\bar{\rho}\,V_{\alpha,i})\right] - \frac{\partial}{\partial \psi_\alpha}\left(\bar{\rho}\tilde{f}S_\alpha(\boldsymbol{\psi})\right)$$

$$V_{\alpha,i} = \begin{cases} \widetilde{D}_{(\alpha)} \dfrac{\partial \widetilde{\Phi}_{(\alpha)}}{\partial x_i} - \tilde{\phi}_\alpha \widetilde{D}_\beta \dfrac{\partial \widetilde{\Phi}_\beta}{\partial x_i} & \text{for species } \alpha \\ \widetilde{D}_{(\alpha)} \dfrac{\partial \widetilde{\Phi}_{(\alpha)}}{\partial x_i} & \text{for enthalpy} \end{cases}$$

Differential diffusion is included

$$\Omega = C_m \frac{\widetilde{D} + \widetilde{D}_T}{\Delta^2}$$

Differential diffusion is not included

A Numerical Challenge

- The modeled transport equation for the joint PDF of composition:

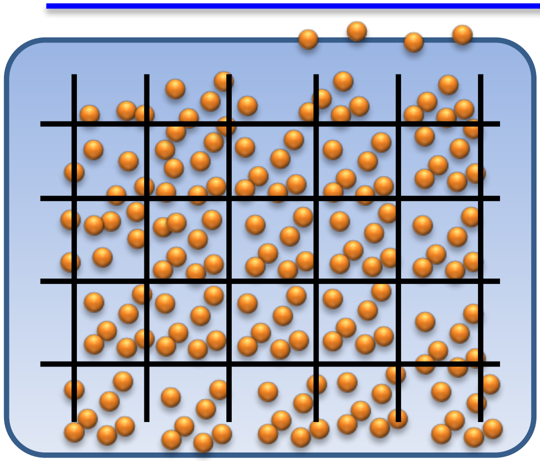
$$\frac{\partial \bar{\rho}\tilde{f}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{f}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\bar{\rho}\,\widetilde{D}_T\,\frac{\partial \tilde{f}}{\partial x_i}\right) = \frac{\partial}{\partial \psi_\alpha}\left[\bar{\rho}\,\tilde{f}\Omega(\psi_\alpha - \tilde{\phi}_\alpha)\right] - \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}\,\frac{\partial}{\partial x_i}(\bar{\rho}\,V_{\alpha,i})\right] - \frac{\partial}{\partial \psi_\alpha}\left(\bar{\rho}\tilde{f}S_\alpha(\boldsymbol{\psi})\right)$$

- The modeled the joint PDF evolves in a high (i.e., $n_s + 4$) dimensional space
  - $n_s = 16$ for a simple CH4/Air combustion with a reduced ARM1 mechanism
  - $n_s = \mathcal{O}(100)$ for a simple Diesel combustion
- Conventional numerical methods (FDM,FVM,FEM, etc.) cannot be used to solve the PDF transport equation
- The remaining alternative is the Monte Carlo method
- Particle-based Lagrangian Monte Carlo method has proved to be a highly effective and viable method (Pope, 1994)
  - Construct an equivalent system of stochastic differential equations.

The Equivalent System

- The modeled transport equation for the joint PDF of composition:

$$\frac{\partial \bar{\rho}\tilde{f}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{f}}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\bar{\rho}\,\widetilde{D}_T\,\frac{\partial \tilde{f}}{\partial x_i}\right)$$
$$= \frac{\partial}{\partial \psi_\alpha}\left[\bar{\rho}\,\tilde{f}\Omega(\psi_\alpha - \tilde{\phi}_\alpha)\right] - \frac{\partial}{\partial \psi_\alpha}\left[\tilde{f}\,\frac{\partial}{\partial x_i}(\bar{\rho}\,V_{\alpha,i})\right] - \frac{\partial}{\partial \psi_\alpha}\left(\bar{\rho}\tilde{f}S_\alpha(\boldsymbol{\psi})\right)$$



The flow is represented by a set of Lagrangian particles.

$$\boxed{\begin{aligned} dX_i &= \left[\tilde{u}_i + \frac{1}{\bar{\rho}}\frac{\partial \bar{\rho}\widetilde{D}_T}{\partial x_i}\right]dt + \sqrt{2\widetilde{D}_T}\,dW_i \\ d\phi_\alpha &= -\Omega(\phi_\alpha - \tilde{\phi}_\alpha)dt + \left(\frac{1}{\bar{\rho}}\frac{\partial \bar{\rho}\,V_{\alpha,j}}{\partial x_j}\right)dt + S_\alpha(\boldsymbol{\phi})dt \end{aligned}}$$

The SDEs exhibit the same joint PDF as that given by the PDF transport equation, i.e., they are equivalent.

The Hybrid Lagrangian/Eulerian Algorithm

- The LES system solved by a FV method:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i}{\partial x_i} = 0$$

$$\frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} + \frac{\partial \bar{\rho}\tilde{u}_i\tilde{u}_j}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial T_{ij}}{\partial x_j}$$

Where

$$\tau_{ij} = \tilde{\mu}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\frac{\partial \tilde{u}_k}{\partial x_k}\delta_{ij}\right); \quad T_{ij} = \bar{\rho}\tilde{u}_i\tilde{u}_j - \bar{\rho}\widetilde{u_i u_j}$$

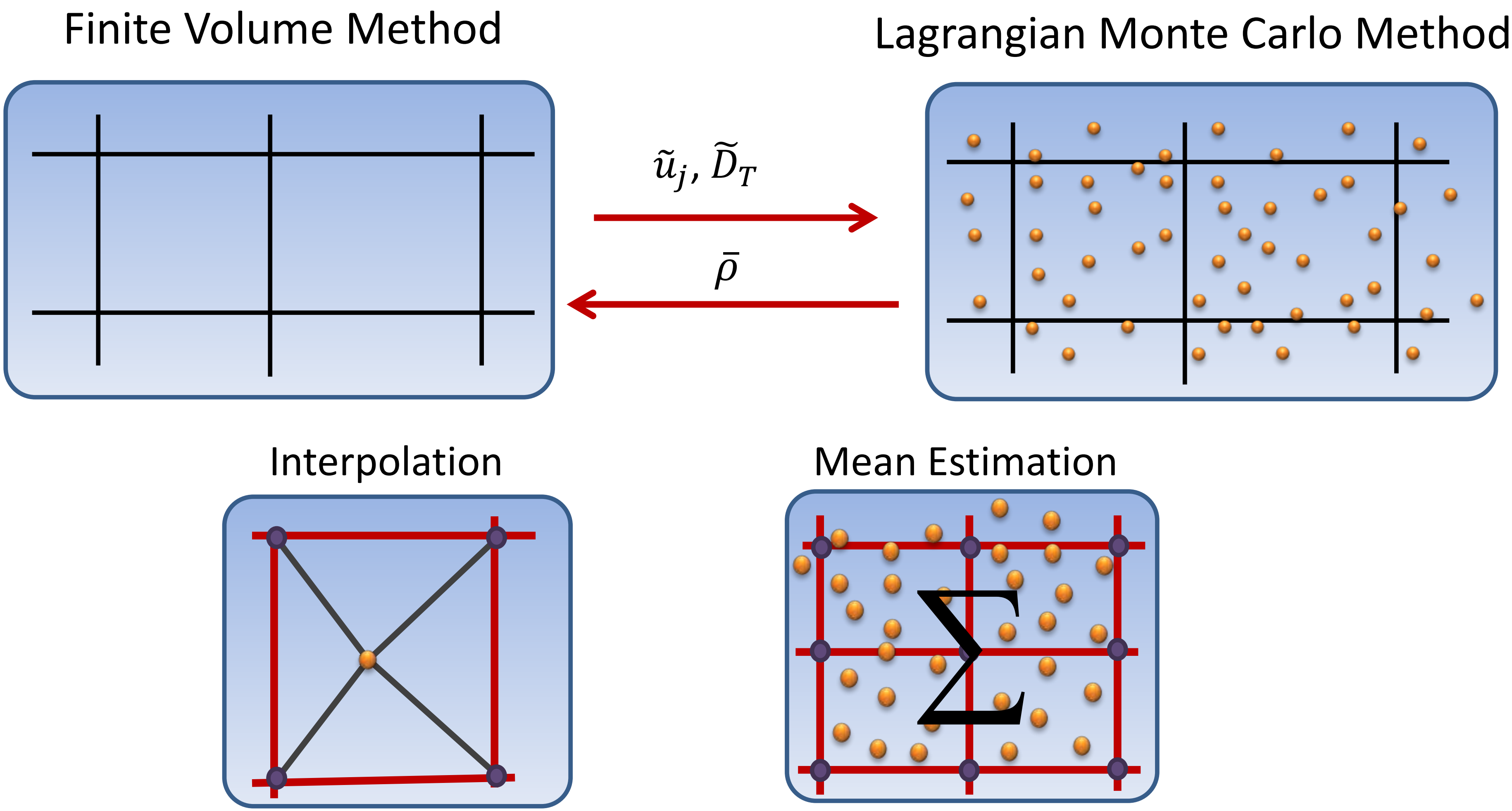
The residual stresses (T_{ij}) are modeled by dynamic Smagorinsky model of Moin et al. (1991) with Lagrangian averaging method of Meneveau et al. (1996)

- The PDF system solved by a Lagrangian Monte Carlo method:

$$dX_i = \left[\tilde{u}_i + \frac{1}{\bar{\rho}}\frac{\partial \bar{\rho}\widetilde{D}_T}{\partial x_i}\right]dt + \sqrt{2\widetilde{D}_T}dW_i$$

$$d\phi_\alpha = -\Omega(\phi_\alpha - \tilde{\phi}_\alpha)dt + \left(\frac{1}{\bar{\rho}}\frac{\partial \bar{\rho}\, V_{\alpha,j}}{\partial x_j}\right)dt + S_\alpha(\boldsymbol{\phi})dt$$

The Numerical Method (Turkeri et al. CTM, 2019)



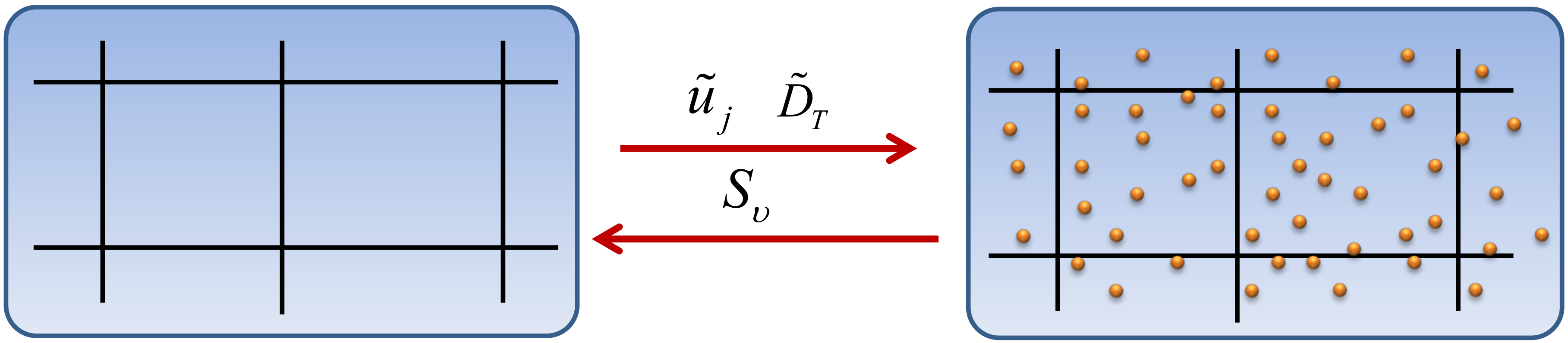
- The LES equations are solved using a FV method (**pimpleFoam**)
- The PDF equations are solved using a Lagrangian Monte Carlo method
- The chemical kinetic equations are solved using **ISAT**

All done in **OpenFAOM**

The Density Coupling (Popov et al. JCP, 2015)

Finite Volume Method

Lagrangian Monte Carlo Method



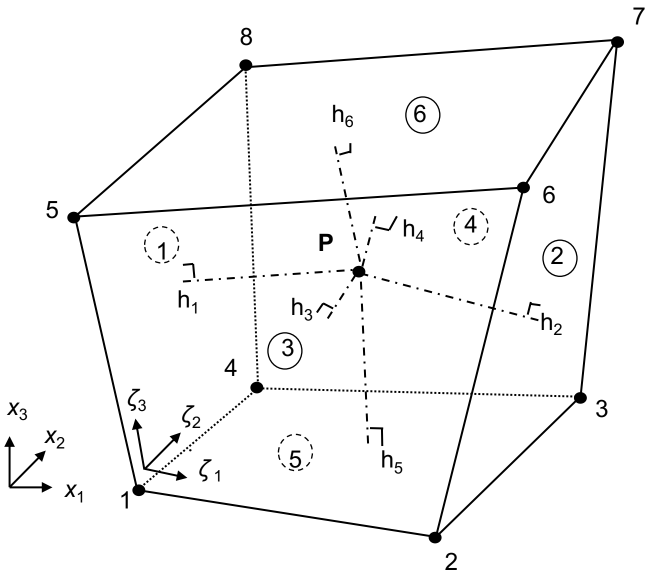
- Using the noisy particle density field in LES causes numerical difficulty
- Instead we ``smooth” the density by solving an equation for specific volume (Popov et al. 2015)

$$\bar{\rho}\frac{\partial \hat{\upsilon}}{\partial t} + \bar{\rho}\frac{\partial \tilde{u}_j \hat{\upsilon}}{\partial x_j} = \bar{\rho}\frac{\partial}{\partial x_j}\left(\tilde{D}_T \frac{\partial \hat{\upsilon}}{\partial x_j}\right) \underbrace{+ S_\upsilon +}_{\text{rate of volume expansion}} \bar{\rho}\,\overbrace{\frac{\tilde{\upsilon}_{PDF} - \hat{\upsilon}}{\tau_\upsilon}}^{\text{relaxation term}}$$

$$\bar{\rho} = \frac{1}{\hat{\upsilon}} \qquad \tau_\upsilon = 4\Delta t$$

The Mean Estimation and Interpolation

Define logical coordinates and basis functions:*



$$\zeta_1 = \frac{h_1}{h_1 + h_2}, \quad \zeta_2 = \frac{h_3}{h_3 + h_4}, \quad \zeta_3 = \frac{h_5}{h_5 + h_6}$$

$$\begin{aligned}
b_1 &= (1-\zeta_1)(1-\zeta_2)(1-\zeta_3), & b_2 &= \zeta_1(1-\zeta_2)(1-\zeta_3), \\
b_3 &= \zeta_1\zeta_2(1-\zeta_3), & b_4 &= (1-\zeta_1)\zeta_2(1-\zeta_3), \\
b_5 &= (1-\zeta_1)(1-\zeta_2)\zeta_3, & b_6 &= \zeta_1(1-\zeta_2)\zeta_3, \\
b_7 &= \zeta_1\zeta_2\zeta_3, & b_8 &= (1-\zeta_1)\zeta_2\zeta_3,
\end{aligned}$$

Mean Estimation*

$$\tilde{\phi}_{(j)} = \frac{\sum_{k\in C_j}\sum_{i=1}^{N^{[k]}} \omega^{(i)}\phi^{(i)} b_\alpha\left(\zeta^{(i)}\right)}{\sum_{k\in C_j}\sum_{i=1}^{N^{[k]}} \omega^{(i)} b_\alpha\left(\zeta^{(i)}\right)}$$

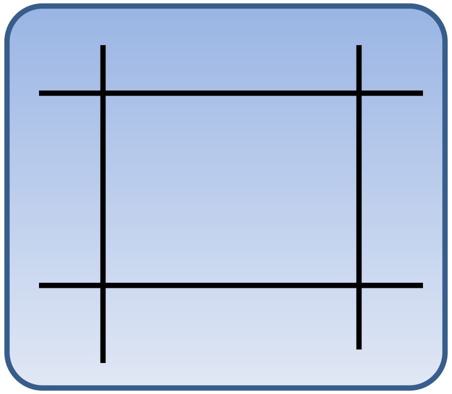
Interpolation onto particle locations*

$$\tilde{\phi}^{(i)} = \sum_\alpha \tilde{\phi}_{(j)} b_\alpha\left(\zeta^{(i)}\right)$$

*Zhang and Haworth, JCP (2004).

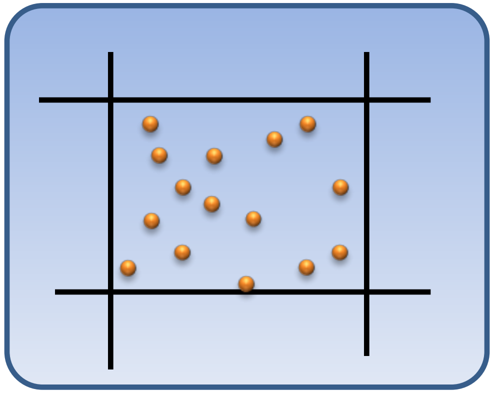
The Consistency Condition*

Finite Volume Method



$$\tilde{\rho}_k = \frac{\sum_{\alpha \in k} m_\alpha}{V_k}$$

Monte Carlo Method



- The density in the FV-LES solver should be equal to the particle mass density in the PDF solver
- This condition should be satisfied throughout the simulations
- A three-stage velocity correction algorithm is employed to enforce the condition

*Muradoglu et al. JCP (2001)

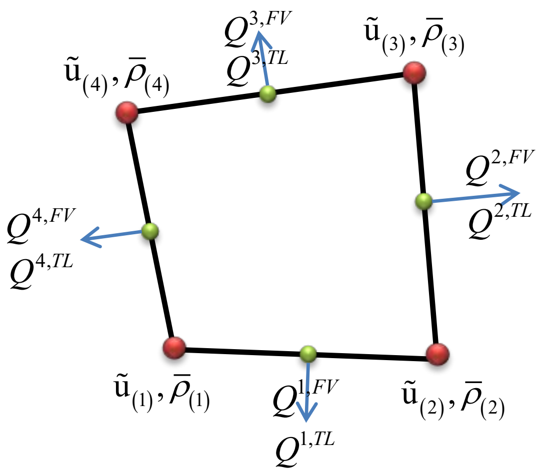
The Velocity Correction*

The Three-Stage Velocity Correction Method*

- The first stage:
  - Linear interpolation from cell centers to cell vertices
- The second stage:
  - A linear system of equations is solved to make the fluxes implied by linear interpolation consistent with FV fluxes
- The third stage: The post correction
  - An equation is solved to eliminate the residuals between FV mass and particles mass

$$R^k \equiv \frac{m^{k,FV} - m^{k,p}}{\tau_{s3}} \text{ where } \tau_{s3=k\Delta t}$$

  - A pressure-Poisson like equation is solved
  - A relaxation is applied to avoid extreme corrections
  - Not usually required

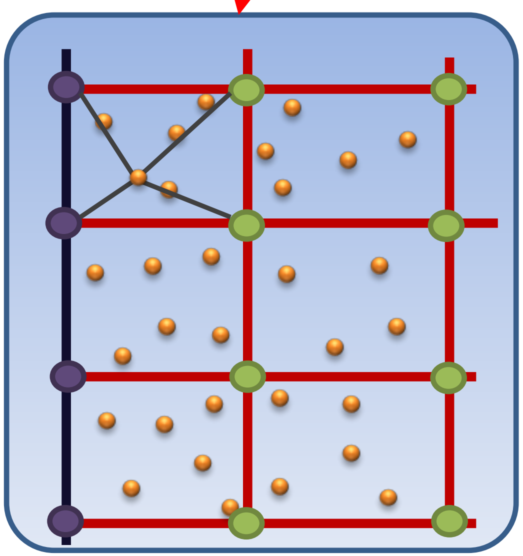


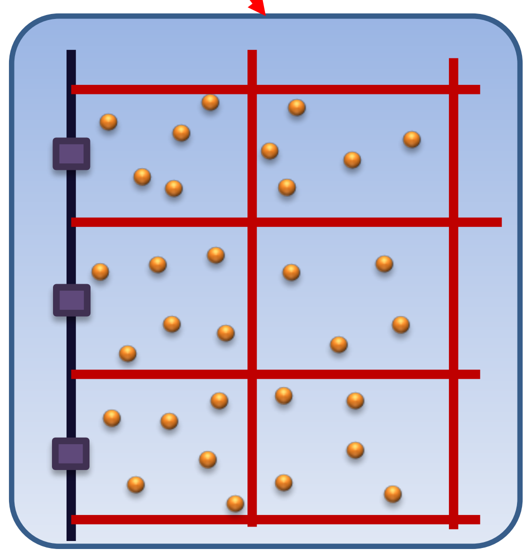
*Zhang and Haworth, JCP (2004) and Turkeri et al. CTM (2019).

Heat Loss Through Walls

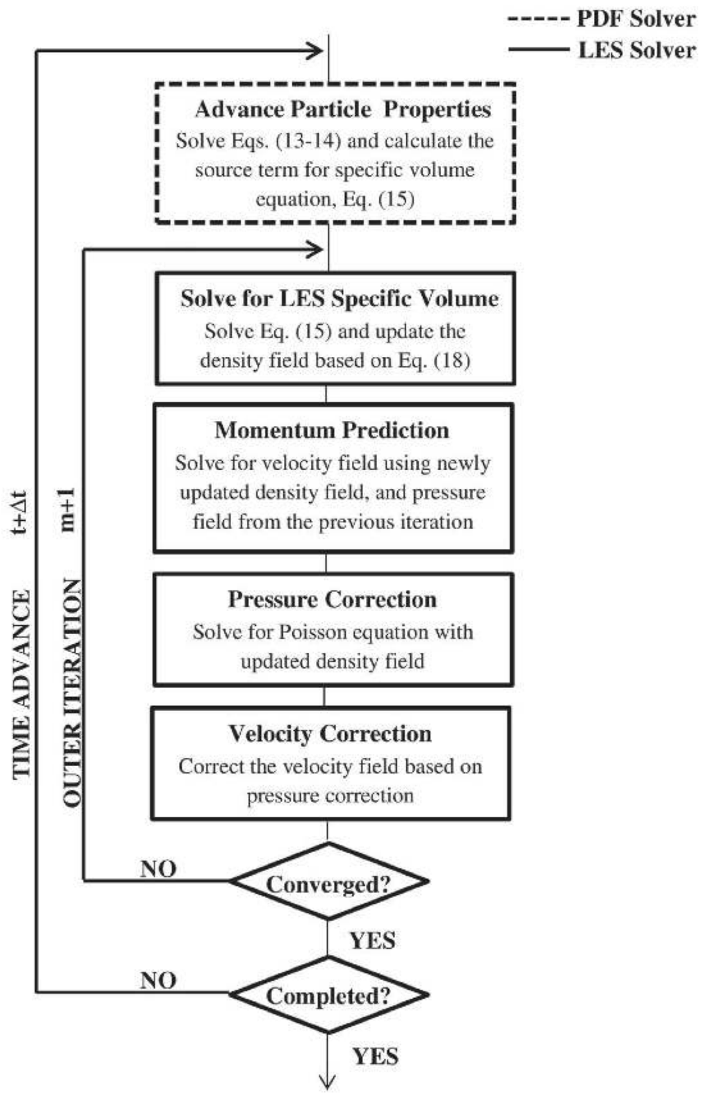
Heat loss through the wall is accounted for through the modification of the mean fields:

$$d\phi_\alpha(t) = -\Omega\left(\phi_\alpha - \boxed{\tilde{\phi}_\alpha}\right)dt + \left(\frac{1}{\bar{\rho}}\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{D}_{(\alpha)}\frac{\partial \boxed{\tilde{\phi}_\alpha}}{\partial x_j}\right)\right)dt + S_\alpha(\phi)dt$$

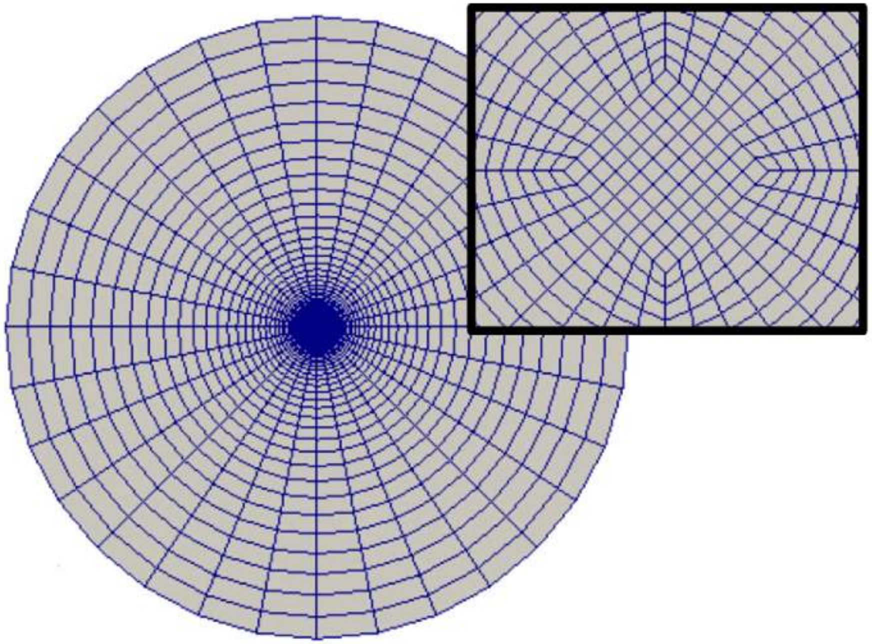




Overall Solution Algorithm*



The flow chart of the LES/PDF solver.



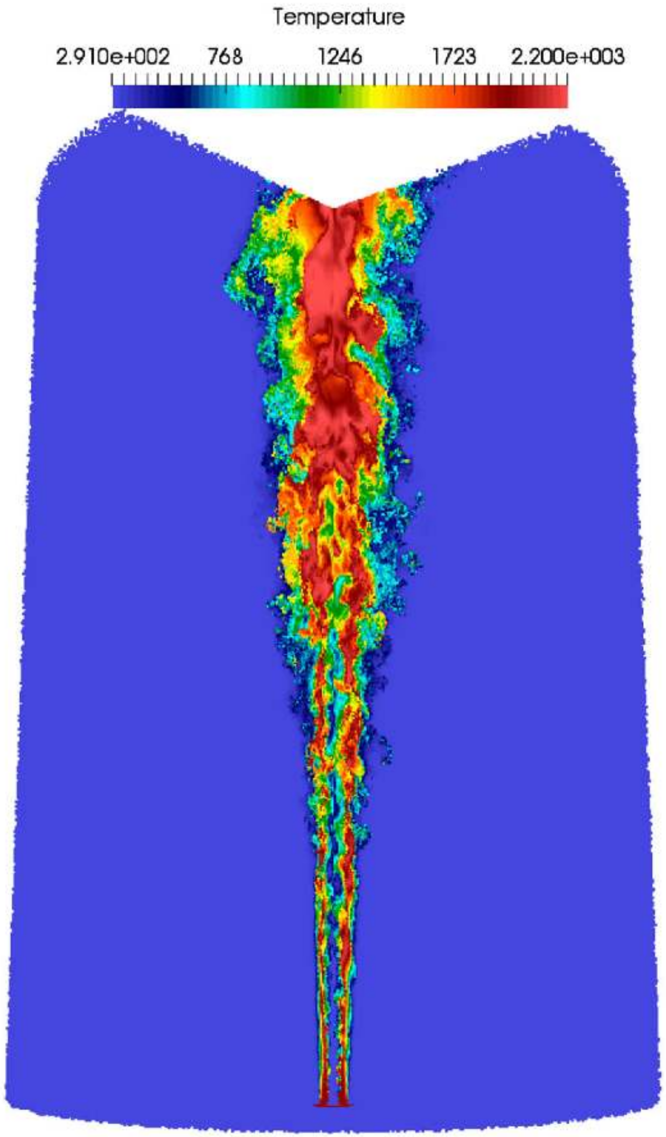
The block-structured grid used in the simulations.

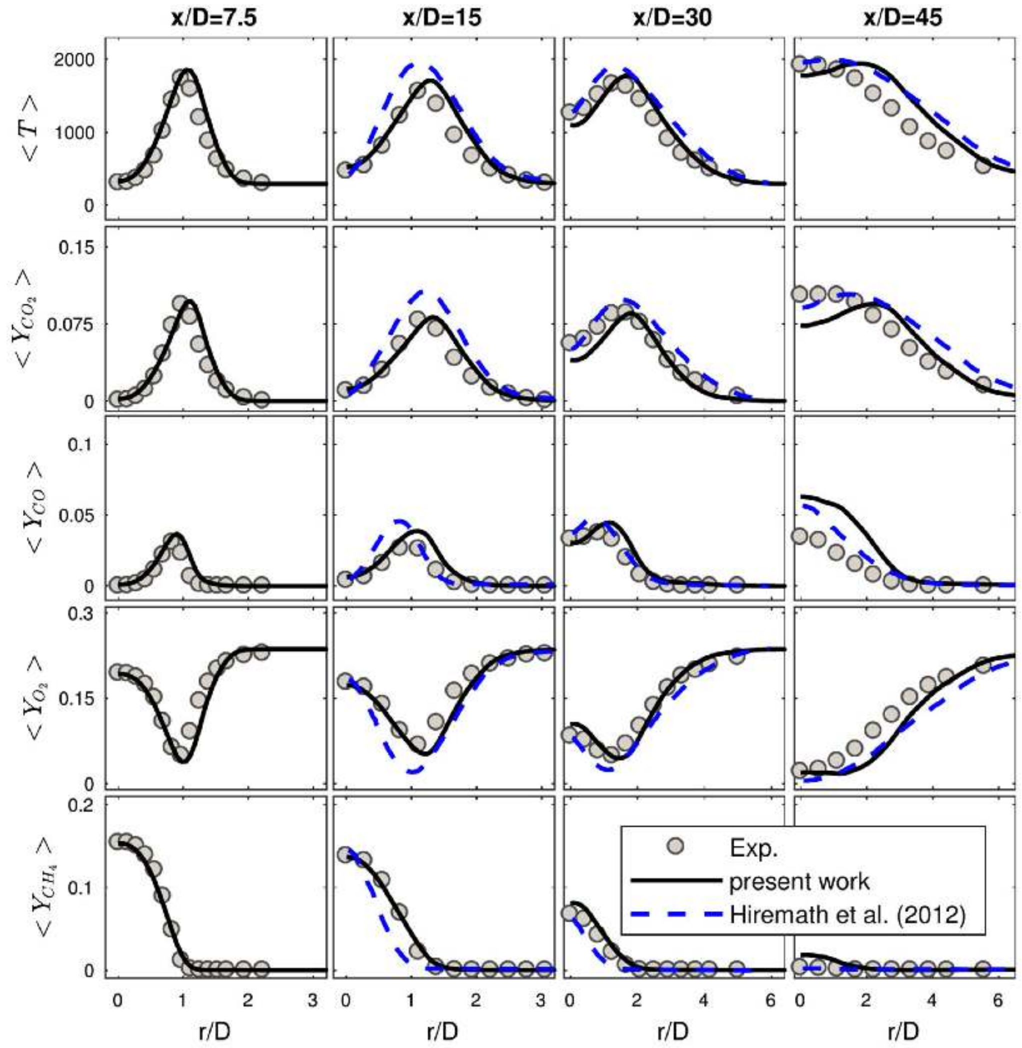
- The present simulations have been performed using block-structured grids
- But the fully unstructured grids can be used in complex geometries
- Can be applied to realistic geometries including industry scale combustors

*Turkeri et al. CTM (2019).

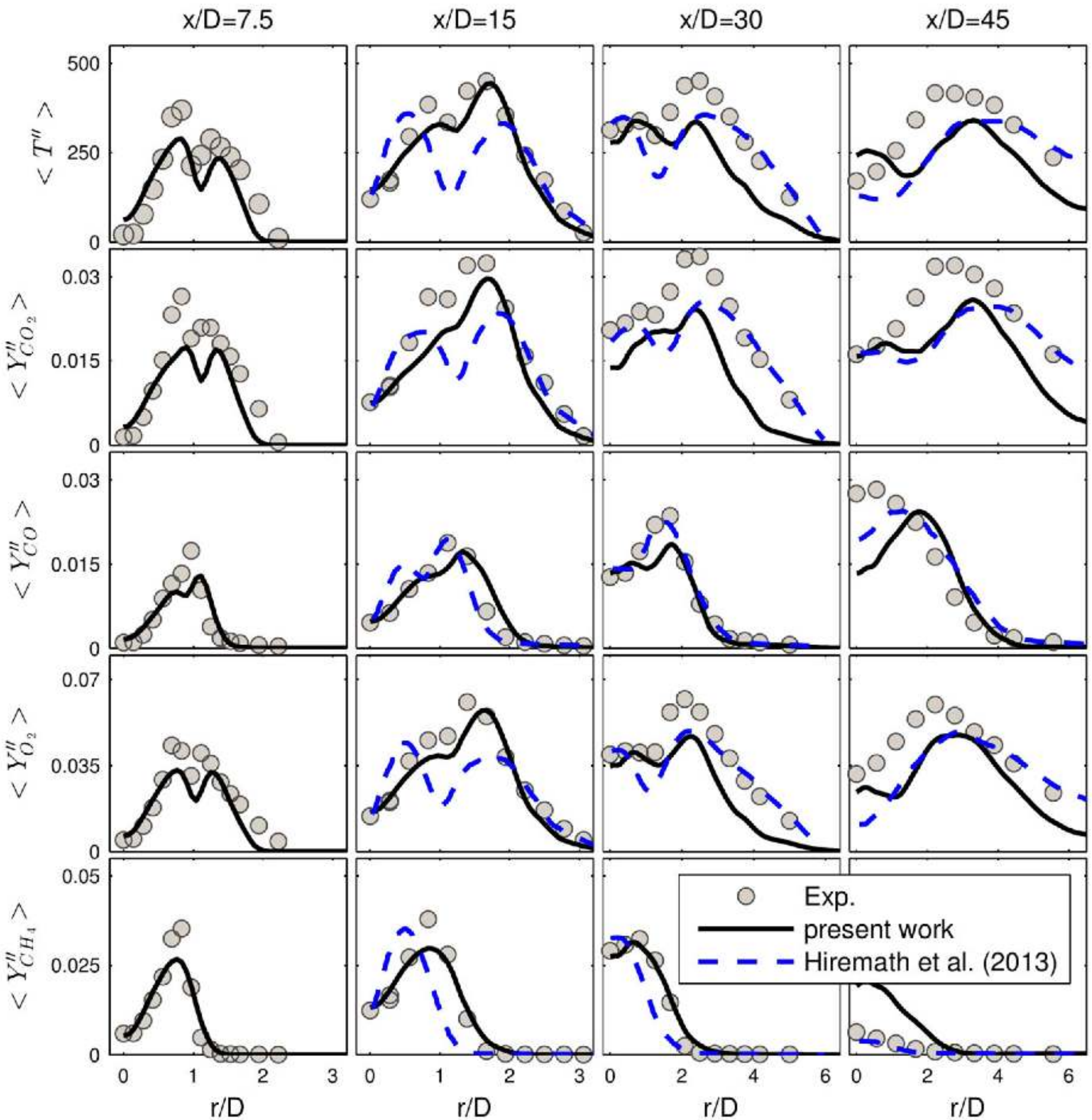
Validation: Sandia Flame-D

Test case: Sandia Flame D with flamelet





Validation: Sandia Flame-D

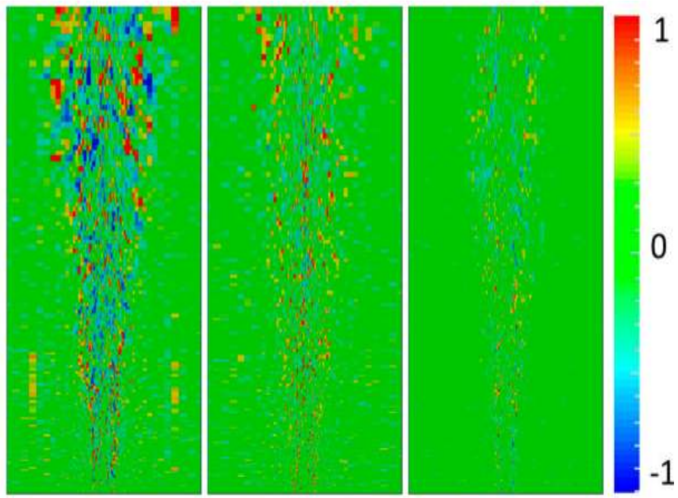


Performance of Velocity Correction Algorithm

Test case: Sandia Flame D with flamelet

Consistent transport equations are solved by both

- FV method in LES solver
- Monte Carlo method in PDF solver

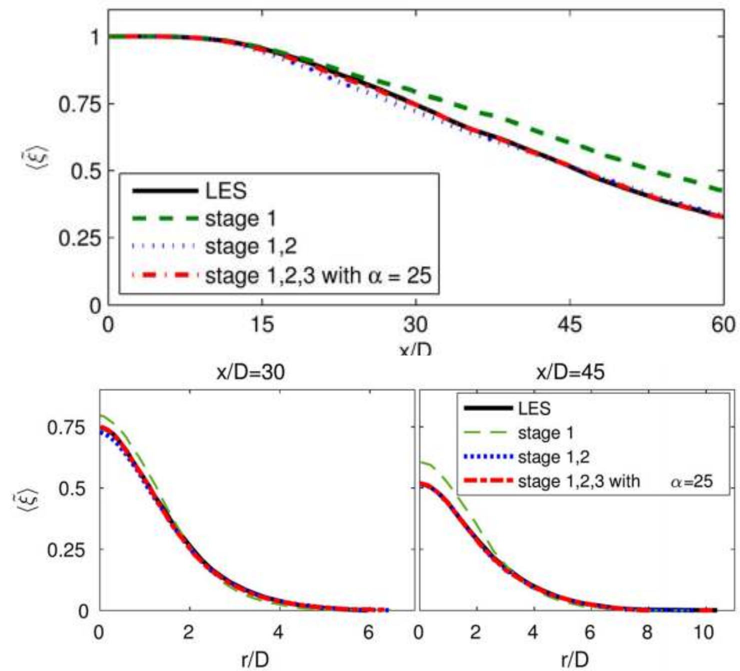


Stage 1 Stage 1,2 Stage 1,2,3

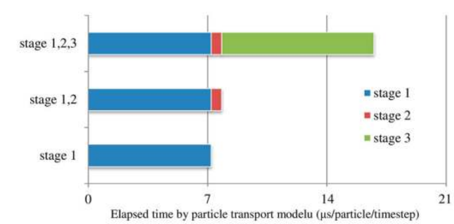
$$R^k \equiv \frac{m^{k,FV} - m^{k,p}}{\tau_{s3}}$$

where $\tau_{s3=k\Delta t}$

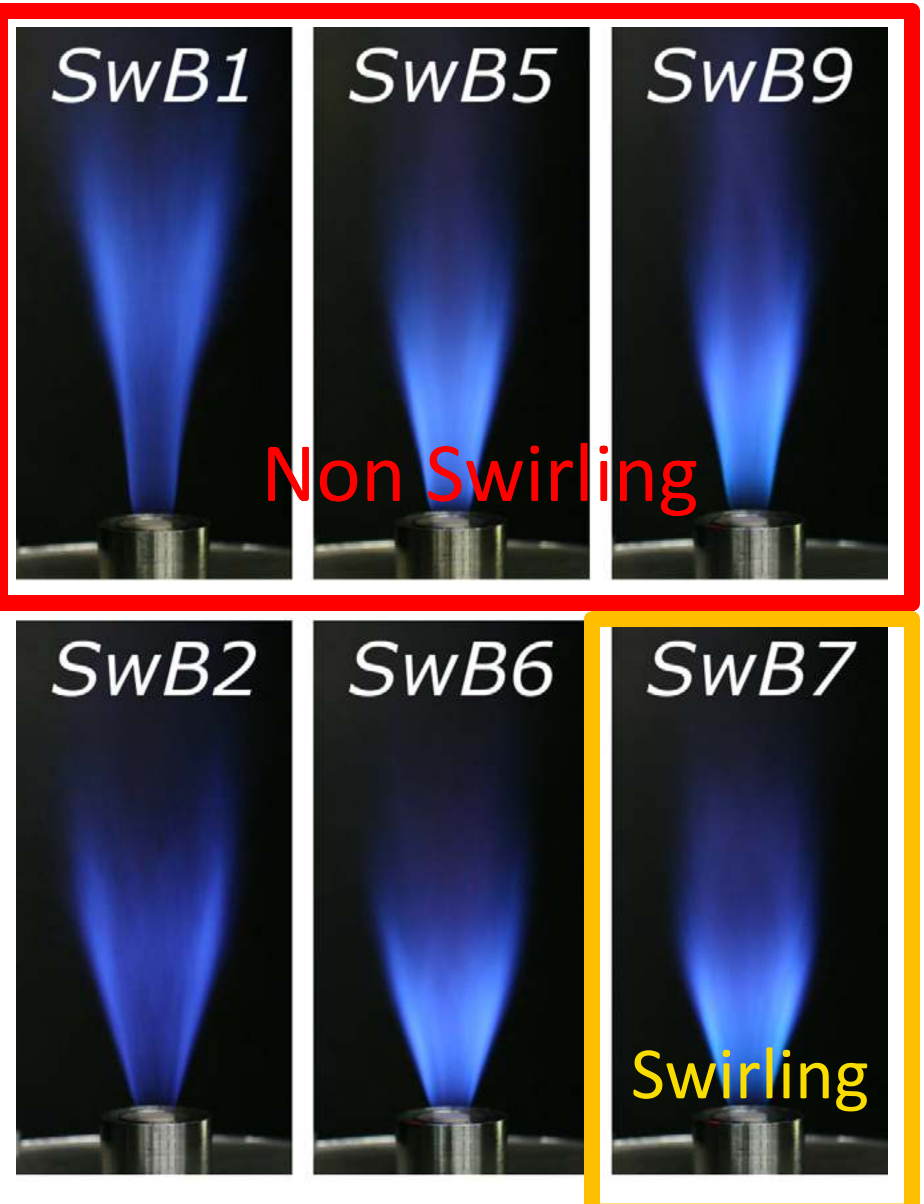
Mean Mixture Fraction



Comp. Cost



Applications: The Cambridge/Sandia Flames*



Operating conditions for Cambridge Stratified Swirl Burner. In all cases $\phi_g = 0.75$, $U_i = 8.31$ m/s, and $U_{co-flow} = 0.4$ m/s. Swirling flows are highlighted in bold font.

Flame	*SFR*	*S*	$\eta(°)$	ϕ_o/ϕ_i	ϕ_i	ϕ_o
SwB1	0	0	0	1	0.75	0.75
SwB2	**0.25**	**0.45**	**24.4**	**1**	**0.75**	**0.75**
SwB3	**0.33**	**0.79**	**38.5**	**1**	**0.75**	**0.75**
SwB5	0	0	0	2	1.0	0.5
SwB6	**0.25**	**0.45**	**24.4**	**2**	**1.0**	**0.5**
SwB7	**0.33**	**0.79**	**38.5**	**2**	**1.0**	**0.5**
SwB9	0	0	0	3	1.125	0.375
SwB10	**0.25**	**0.45**	**24.4**	**3**	**1.125**	**0.375**
SwB11	**0.33**	**0.79**	**38.5**	**3**	**1.125**	**0.375**

*Sweeney et al. CNF, 159 (2012)

Results

Cambridge-Sandia Stratified Non-Swirling Flames

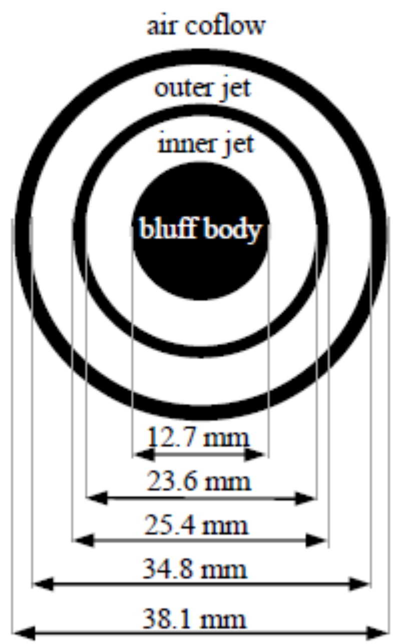
H. Turkeri, X. Zhao, S.B. Pope and M. Muradoglu
"Large eddy simulation/probability density function simulations of the Cambridge turbulent stratified flame series", *Combustion and Flame,* 199:24-45 (2019).

Cambridge Stratified Flame Series: Non-Swirling

Designed to investigate the effects of stratification under non-swirling conditions [1,2,3]

Inlet	Bulk velocity [m/s]	Reynolds number
inner	8.31	5960
outer	18.7	11500
coflow	0.4	-

	$Ø_i$	$Ø_o$	$Ø_i/Ø_o$
SwB1	0.75	0.75	1
SwB5	1	0.5	2
SwB9	1.125	0.375	3



	Computational Details
Domain	200mm x 200mm x 2π
Mesh	2.3 millioncells
Time step	2x 10^{-6} s
PDF Particles	20 per cell
Cost	380 μs/cell/core/time step

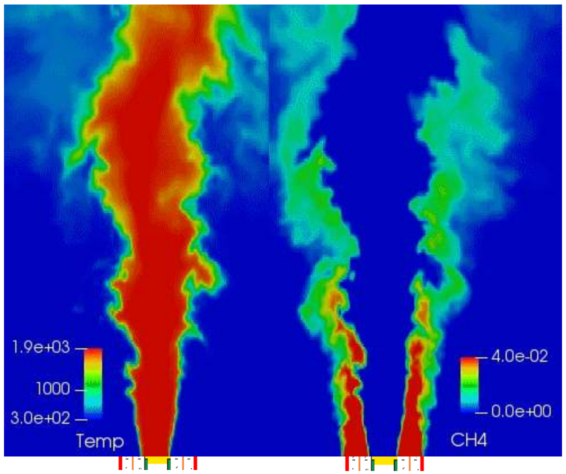
[1] - Sweeney et al., Combust. Flame, 2012 .
[2] - Sweeney et al., Combust. Flame, 2012.
[3] - Zhou et al., Combust. Flame, 2012.

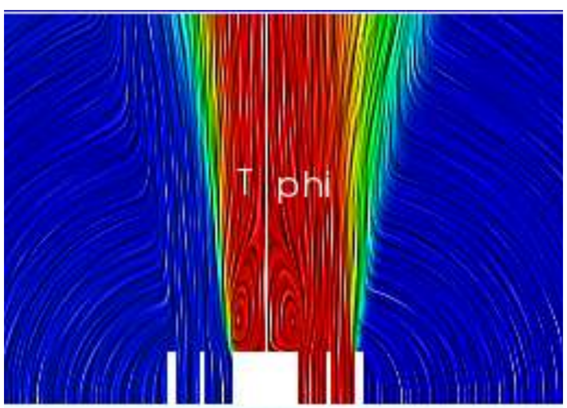
Model variations for parametric studies.

Model	C_m mixing coefficient	Differential diffusion	SwB1	SwB5	SwB9
DD25	25	✓	✓	✓	✓
DD50	50	✓	✗	✓	✗
ED25	25	✗	✓	✓	✓

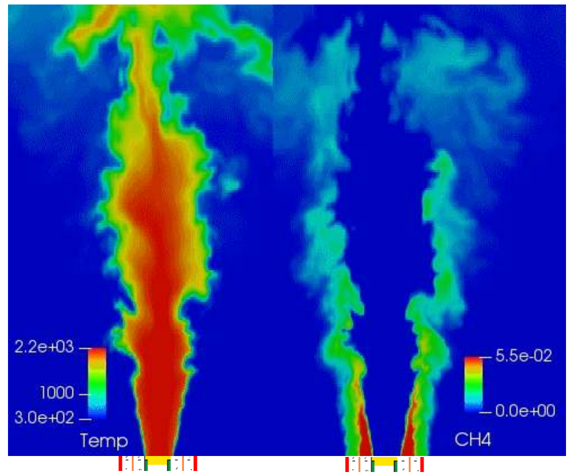
Cambridge Stratified Flames: Non-swirling cases

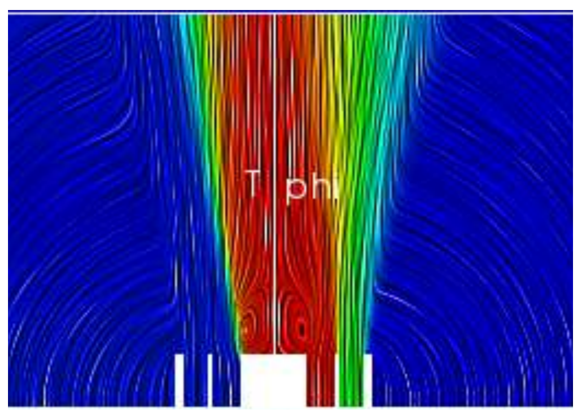
Premixed Flame
(SwB1)



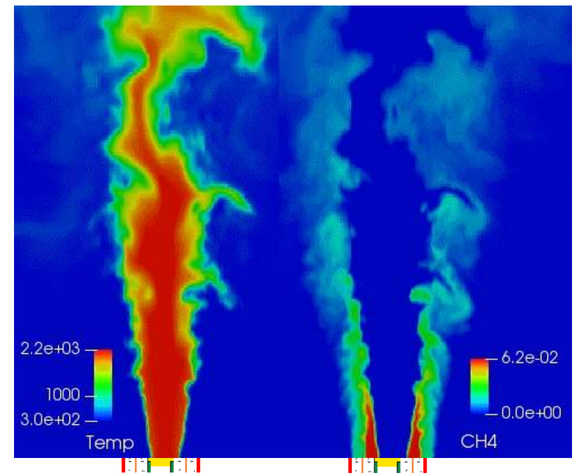


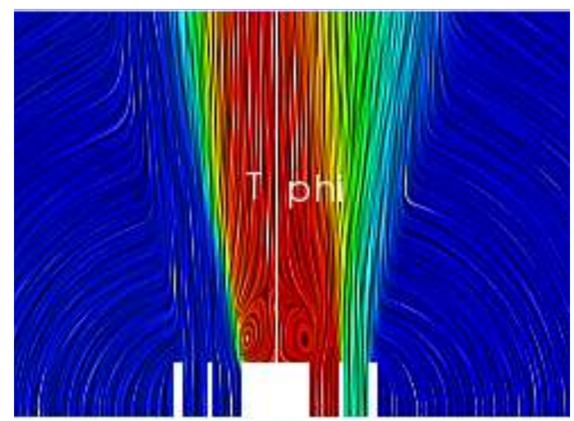
Moderately Stratified Flame
(SwB5)





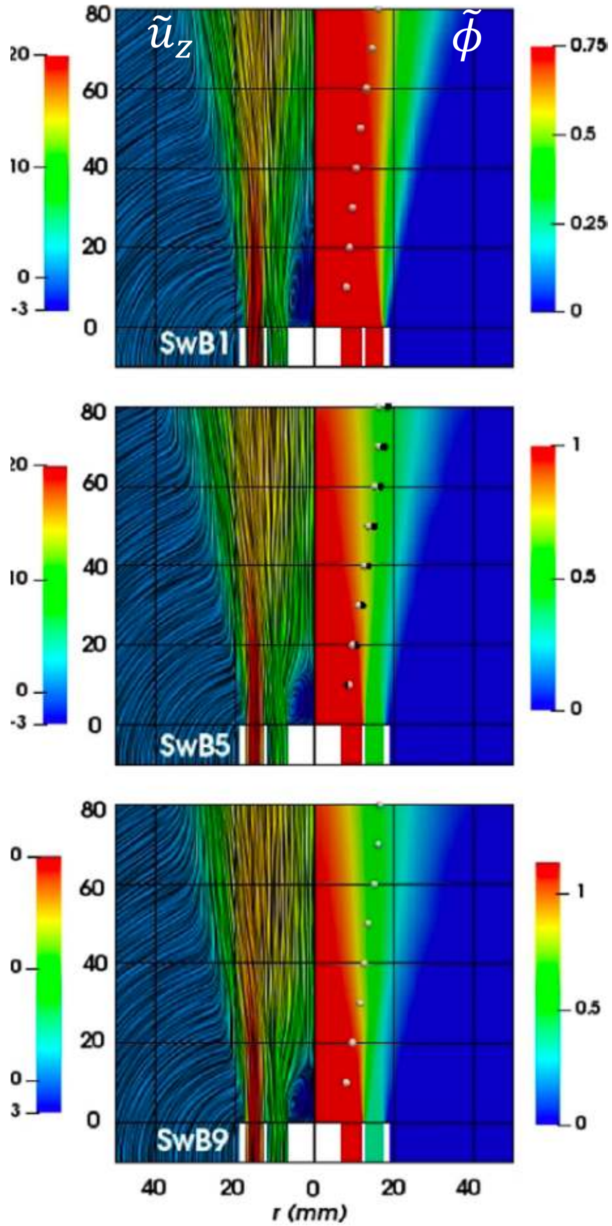
Highly Stratified Flame
(SwB9)

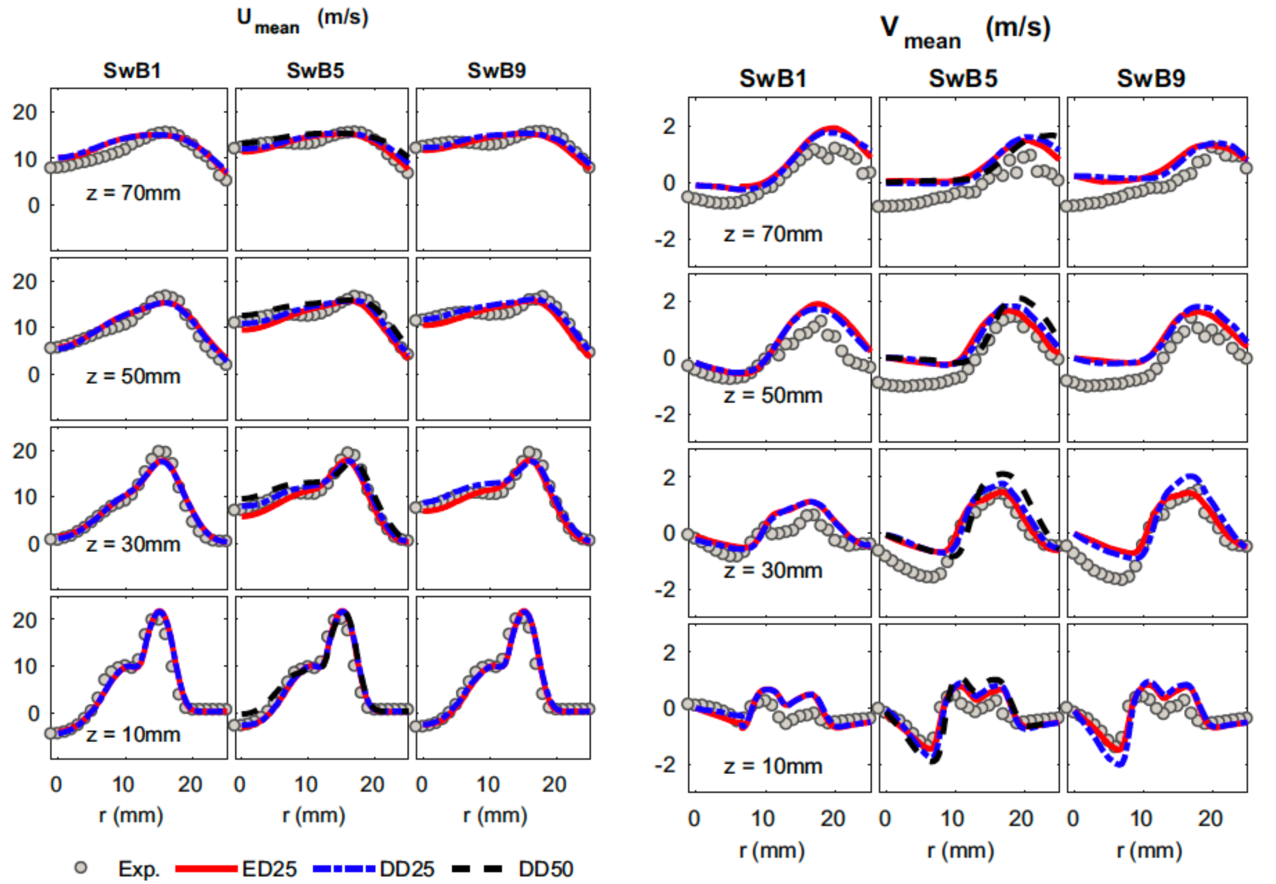




[1] H. Turkeri, X. Zhao, S. B. Pope and M. Muradoglu, Combustion and Flame, 2019.

Numerical Results: Mean Velocity Profiles

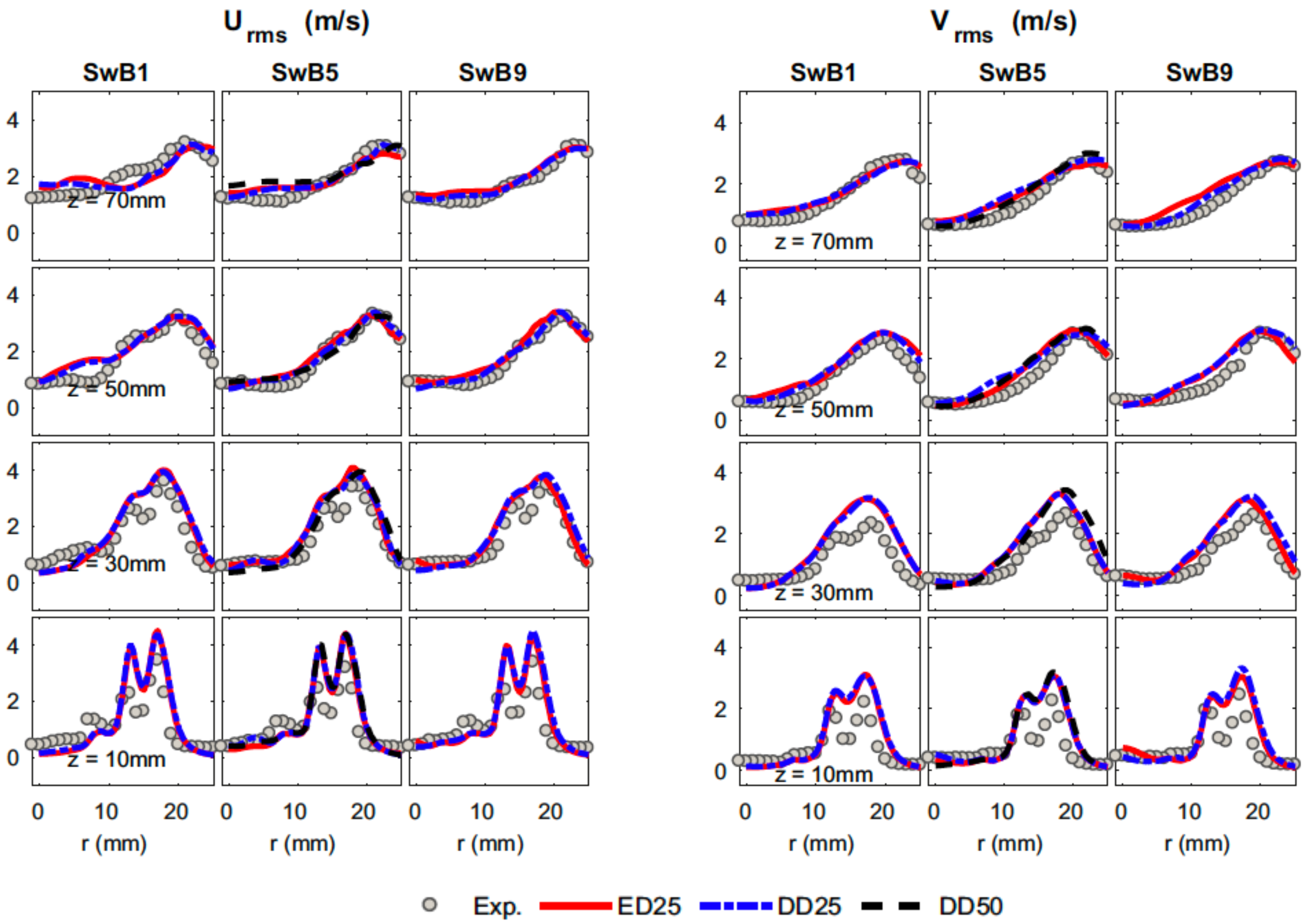




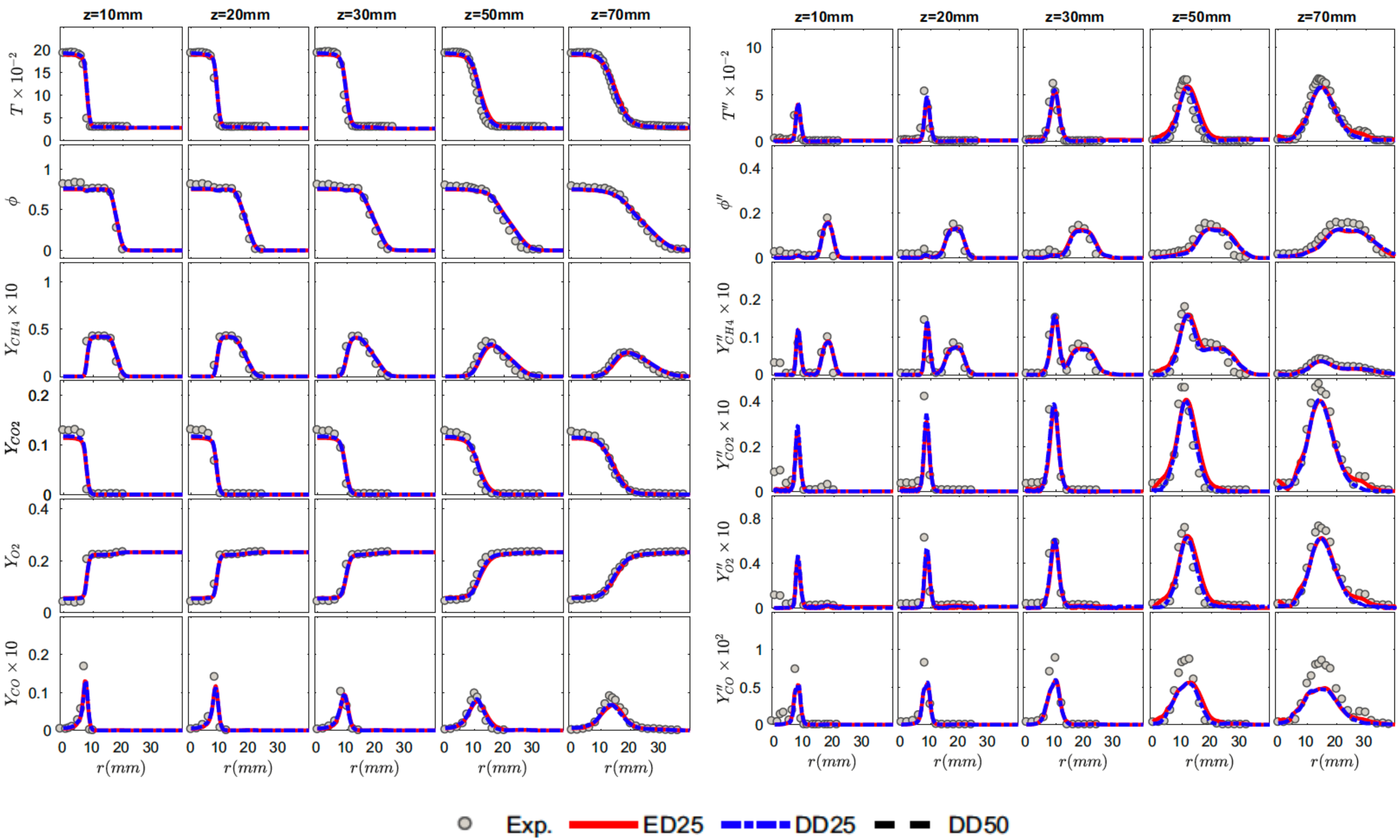
The length of recirculation zones (mm).

Case	DD25	ED25	DD50	Exp.
SwB1	23	23.25	–	24
SwB5	13.5	14	10	14.5
SwB9	14	14.5	–	15

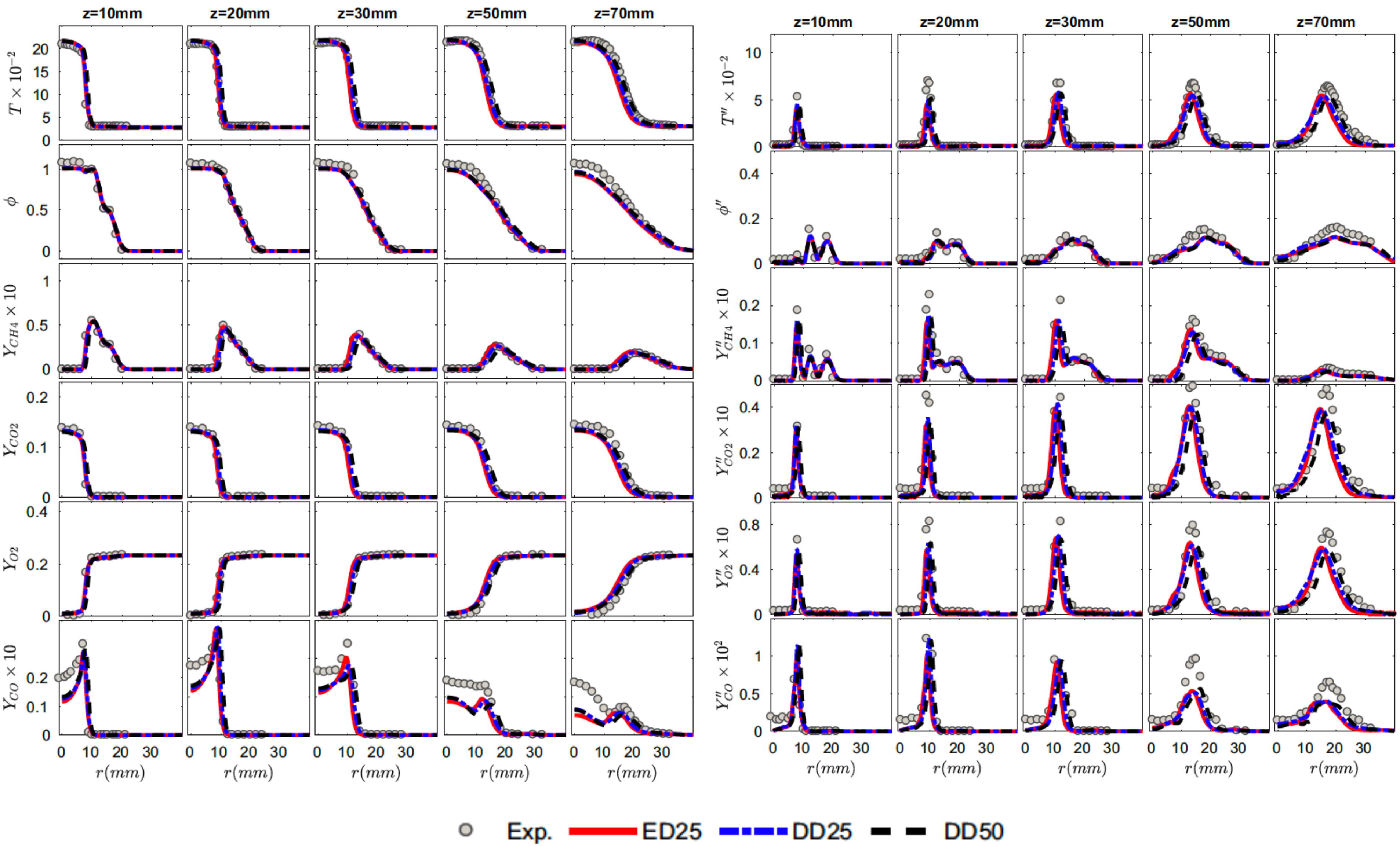
Numerical Results: RMS Velocity Profiles



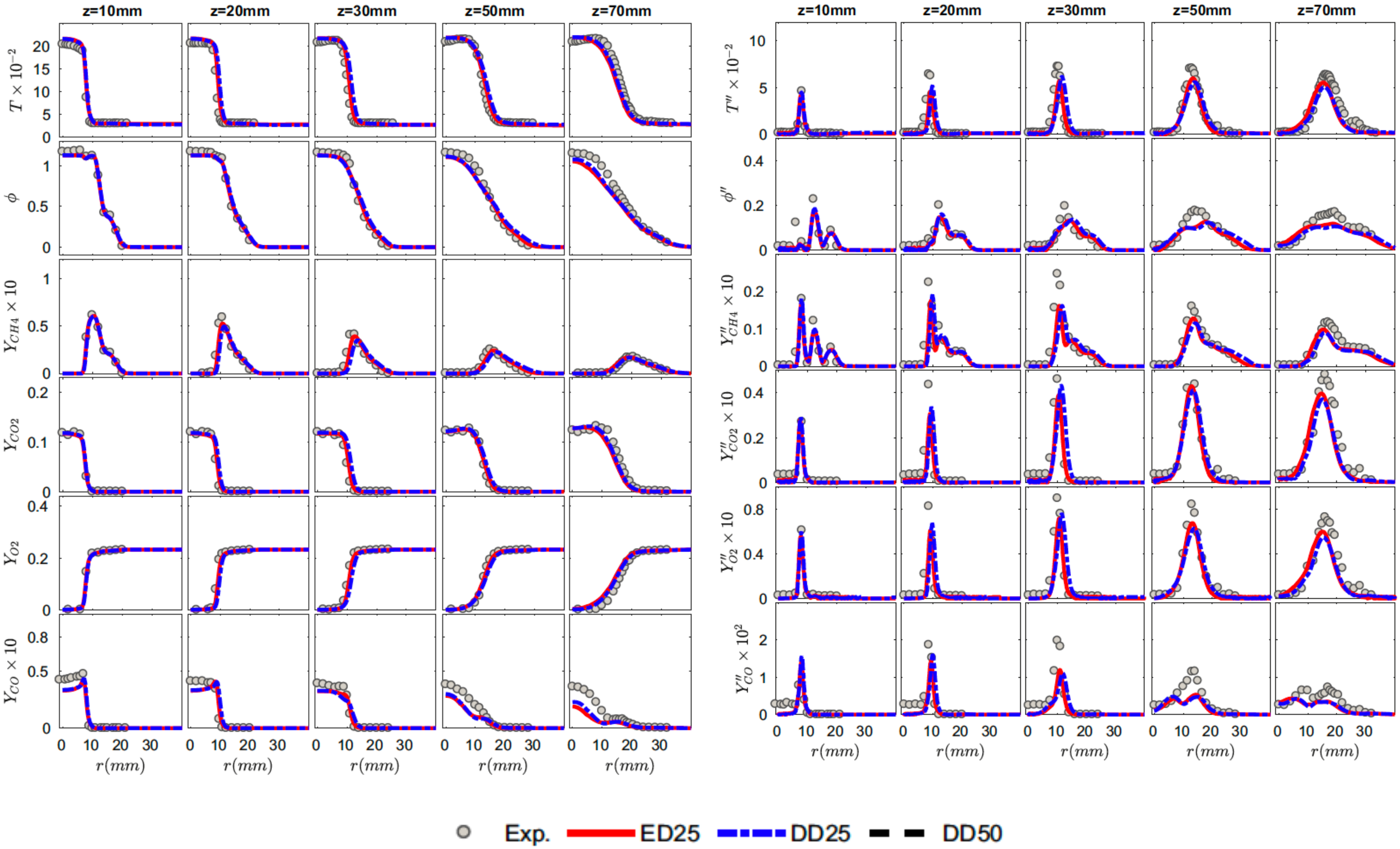
Scalar Fields– SwB1 (Premixed)



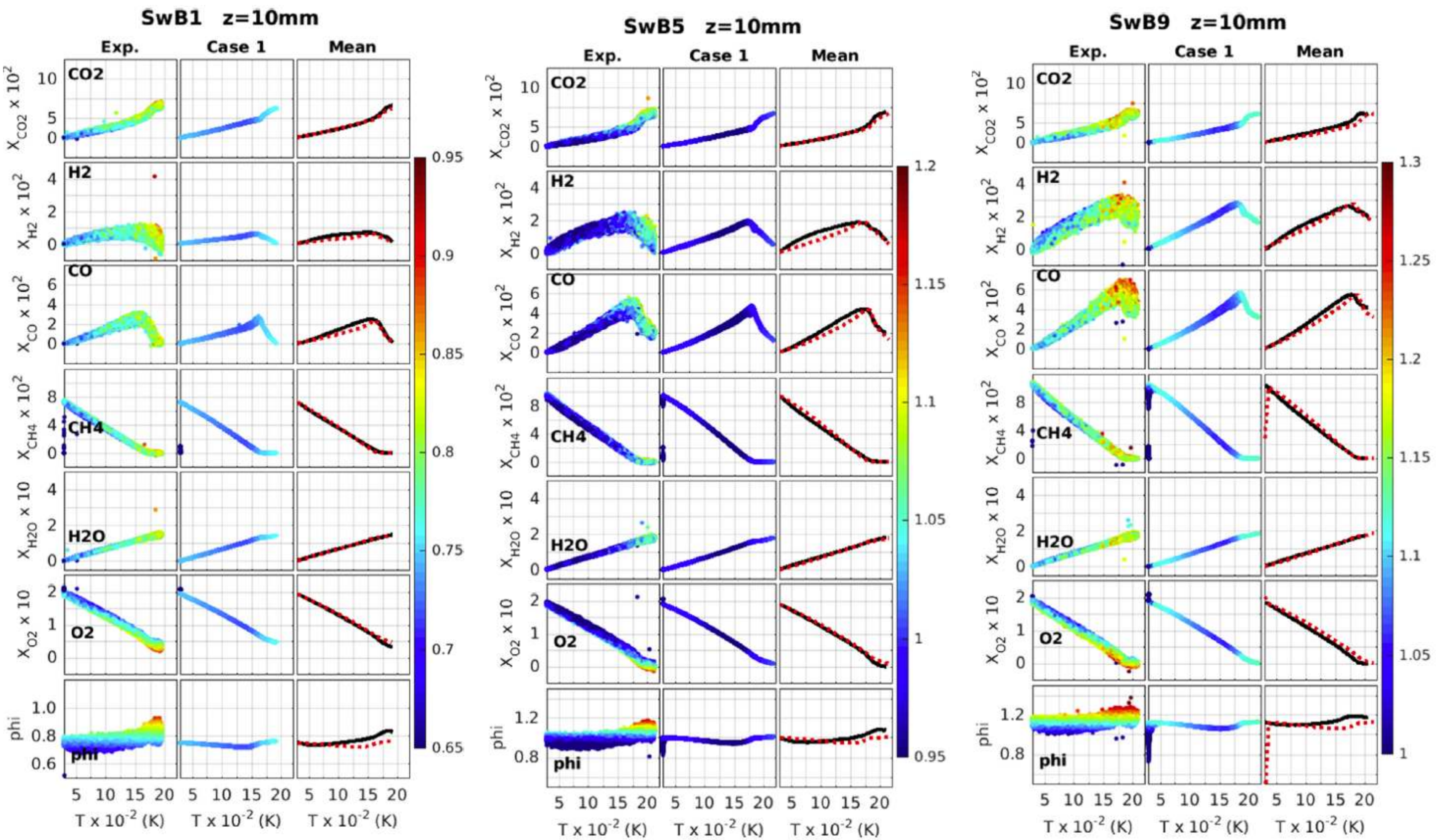
Scalar Fields– SwB5 (Moderately Stratified)



Scalar Fields– SwB9 (Highly Stratified)

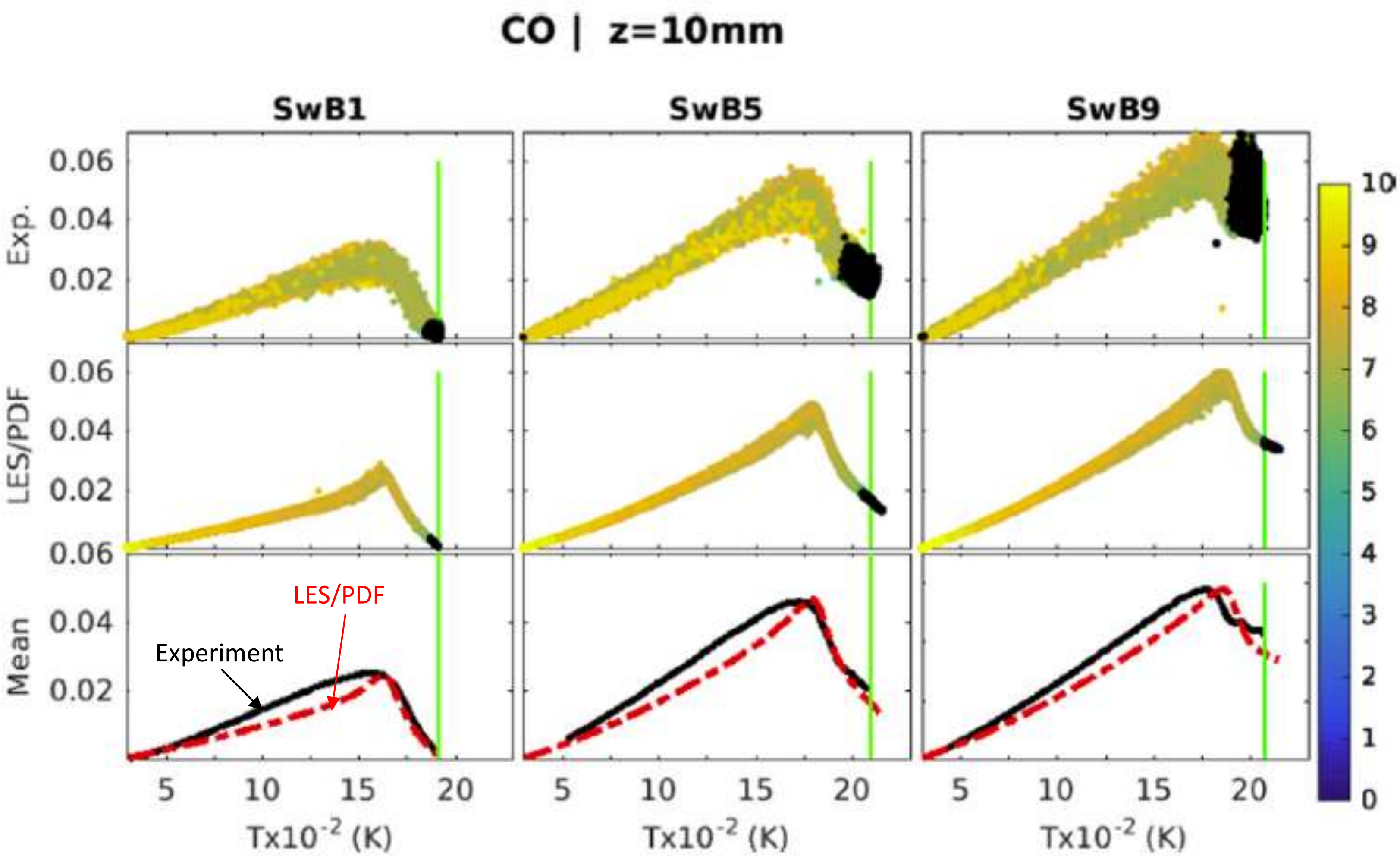


Scatter Plots



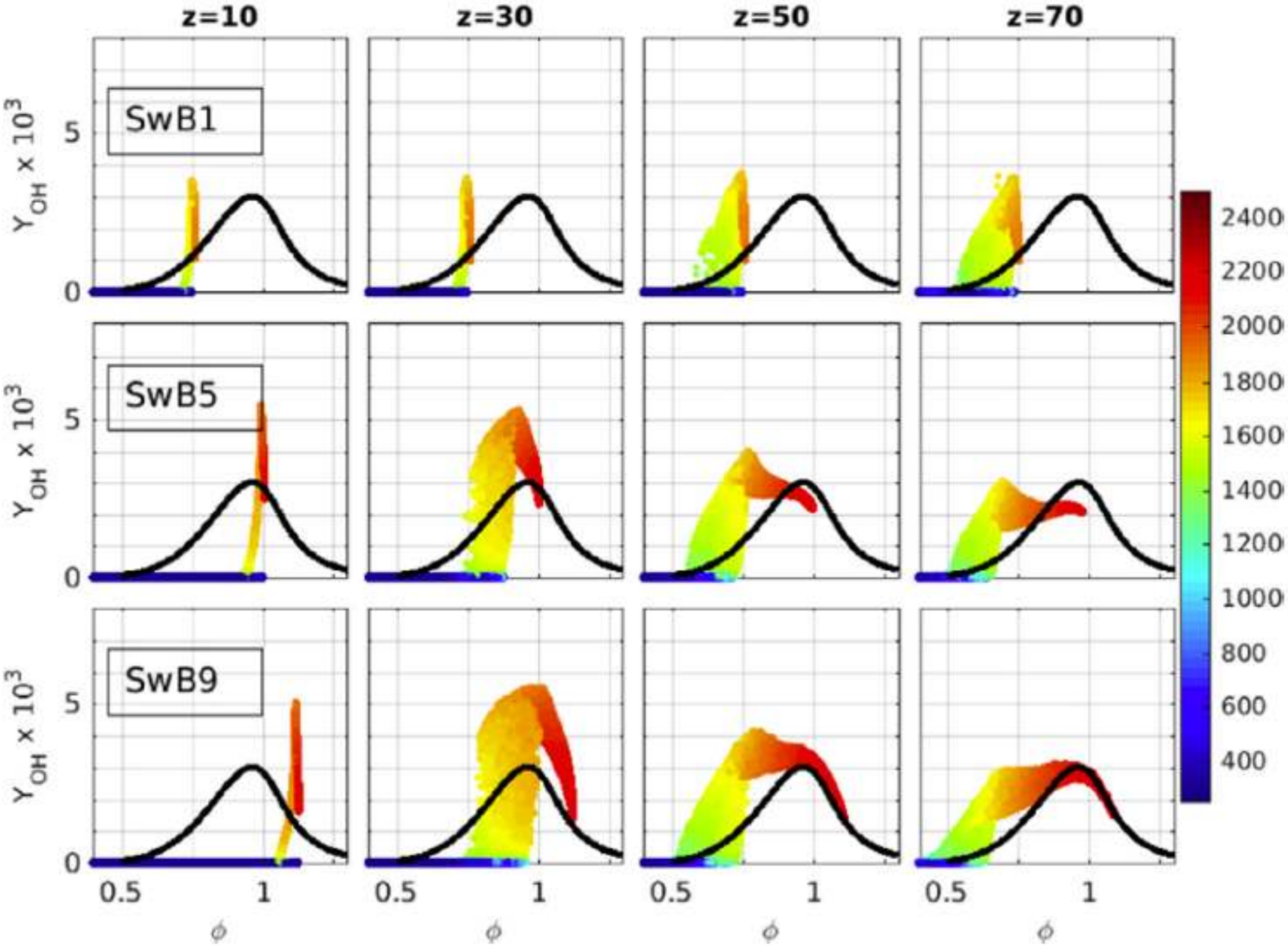
Color-coded by the equivalence ratio. Lines: Conditional mean; Black solid: Exp. Red dotted: comput.

Scatter Plots of CO



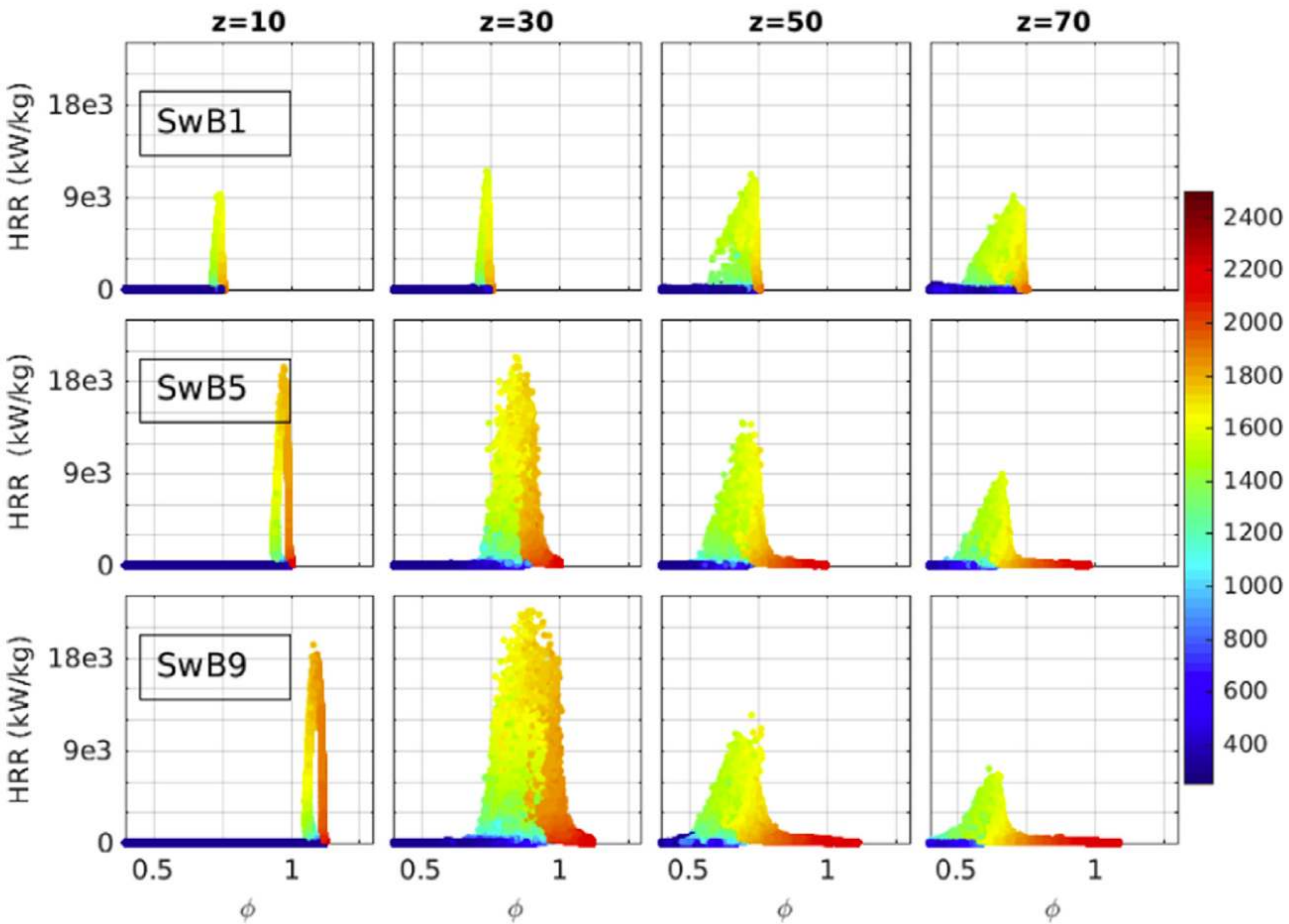
- Color-coded by radial distance
- Black dots: Particles in the recirculation zone, i.e., radial distance < 5 mm
- Black line: Experimental data
- Red line: LES/PDF simulations

Effect of stratification (Model: DD25)

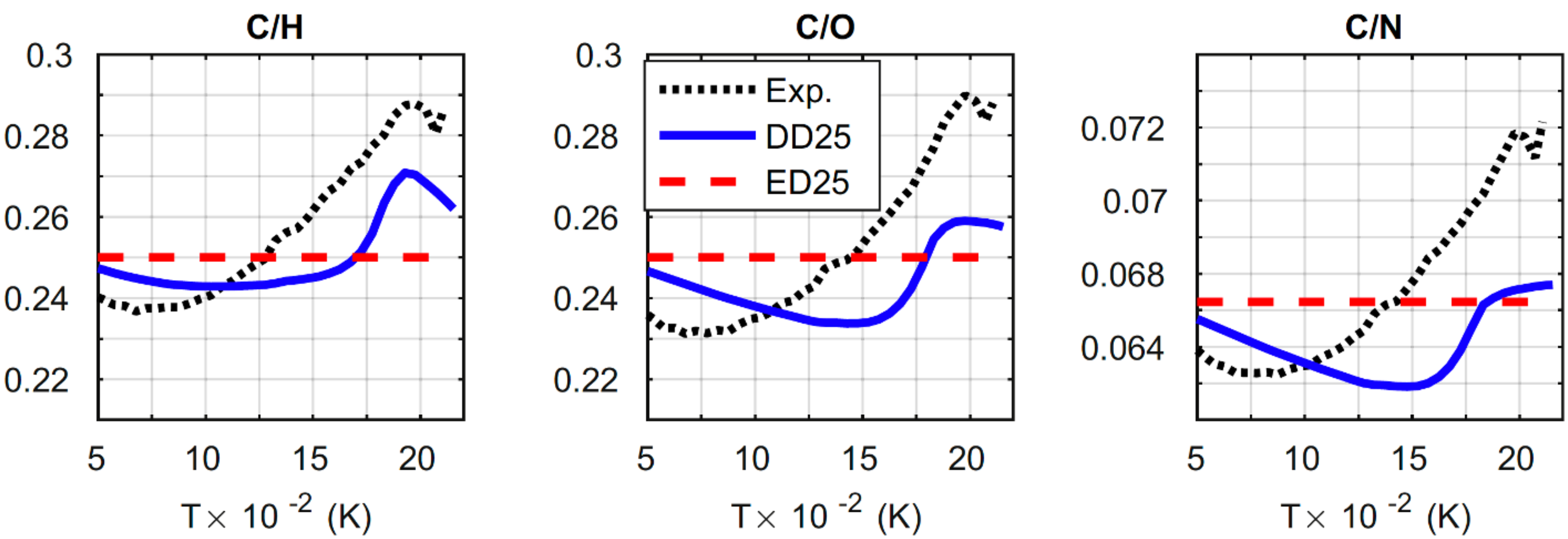


Solid Lines: The OH as a function of the equivalence ratio obtained from the chemical equilibrium calculation. Color-coded by temperature. Model: DD25

Effects of Stratification on Heat Release Rate (HRR)



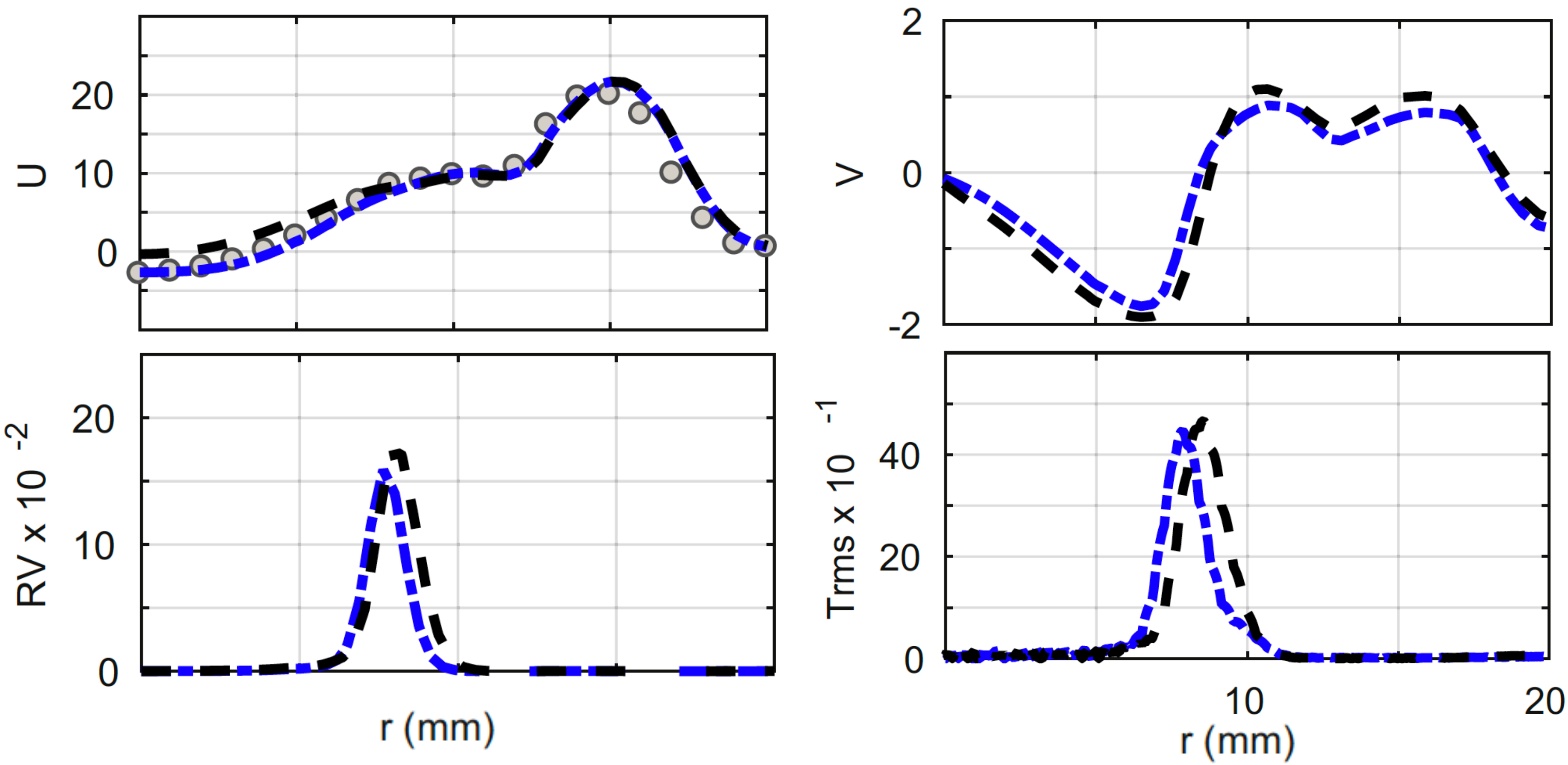
Effects of Differential Diffusion



The atom ratios C/H, C/O and C/N for the moderately stratified case of SwB5.

Dashed Red Line (ED25): Differential diffusion is off
Blue Solid Line (DD25): Differential diffusion is on
Black Dotted Line: Experimental data

Effects of C_m (SwB5)



Blue Dash-Dotted Lines: $C_m = 25$

Black Dashed Lines: $C_m = 50$

Symbols: Experiment

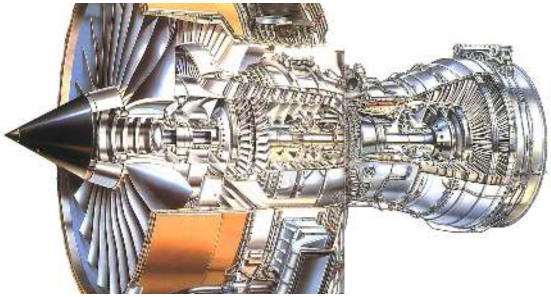
RV = The mean rate of change of specific volume due to mixing and reaction

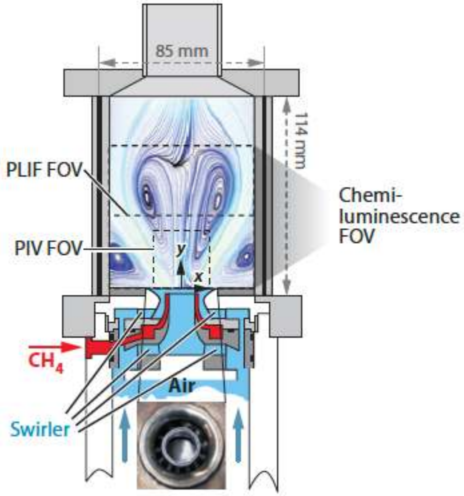
Swirling Flames

Cambridge-Sandia Stratified Swirling Flames

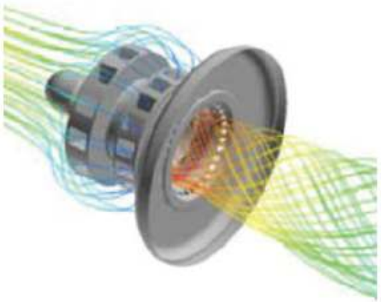
Swirling Flames

- Swirling flow is widely used to stabilize lean premixed turbulent flames in gas turbines to satisfy the low-emission restrictions and to reduce the size of the devices by increasing the residence time.





Steinberg et al. (2010)



Penanhoat (2006)

Objectives:

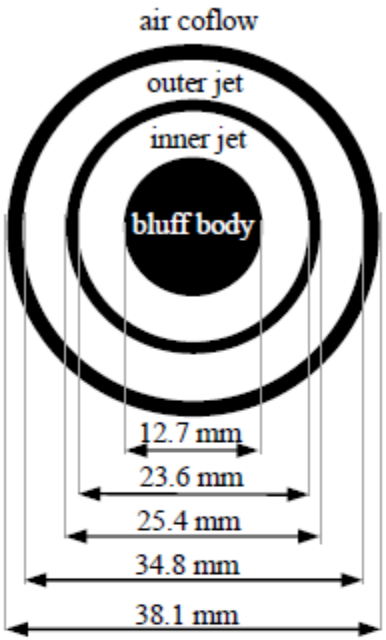
- To assess the predictive capability of the LES/PDF methodology for stratified non-swirling and swirling flames.
- To examine the effect of heat lose through the bluff body

Cambridge Stratified Flame Series

Designed to investigate the effects of stratification under swirl conditions [1,2,3]

Inlet	Bulk velocity [m/s]	Reynolds number
inner	8.31	5960
outer	18.7	11500
coflow	0.4	-

	$\O_i$ / $\O_o$	U_{tg} / U_z
SwB3	1	0.45
SwB7	2	0.45
SwB11	3	0.45

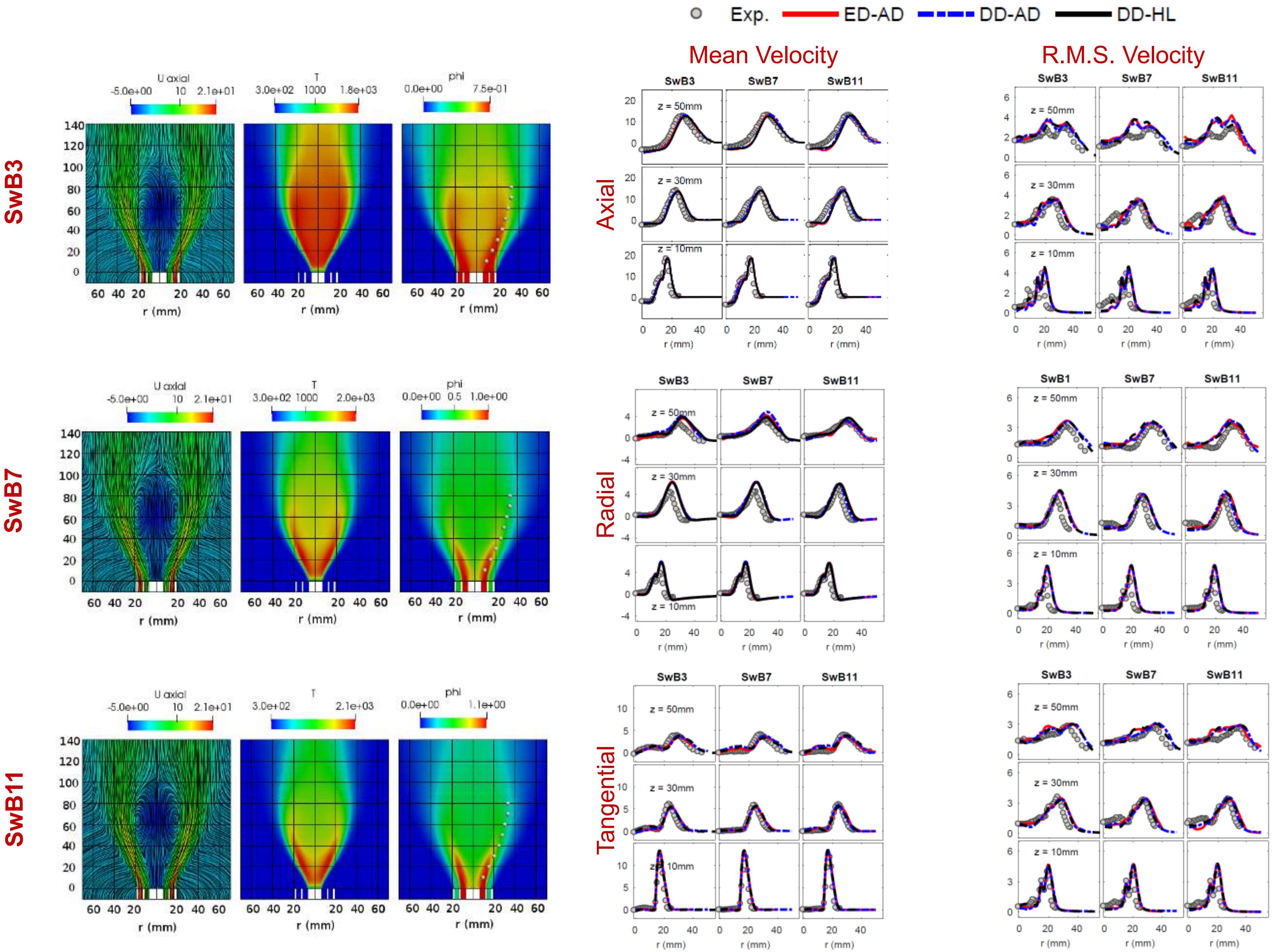


	Computational Details
Domain	300mm x 200mm x 2π
Mesh	2.3 million cells
Time step	2x 10^{-6} s
PDF Particles	20 per cell
Cost	380 μs/cell/core/time step
Chemistry	16-species ARM1
Diffusion	Equal and Differential

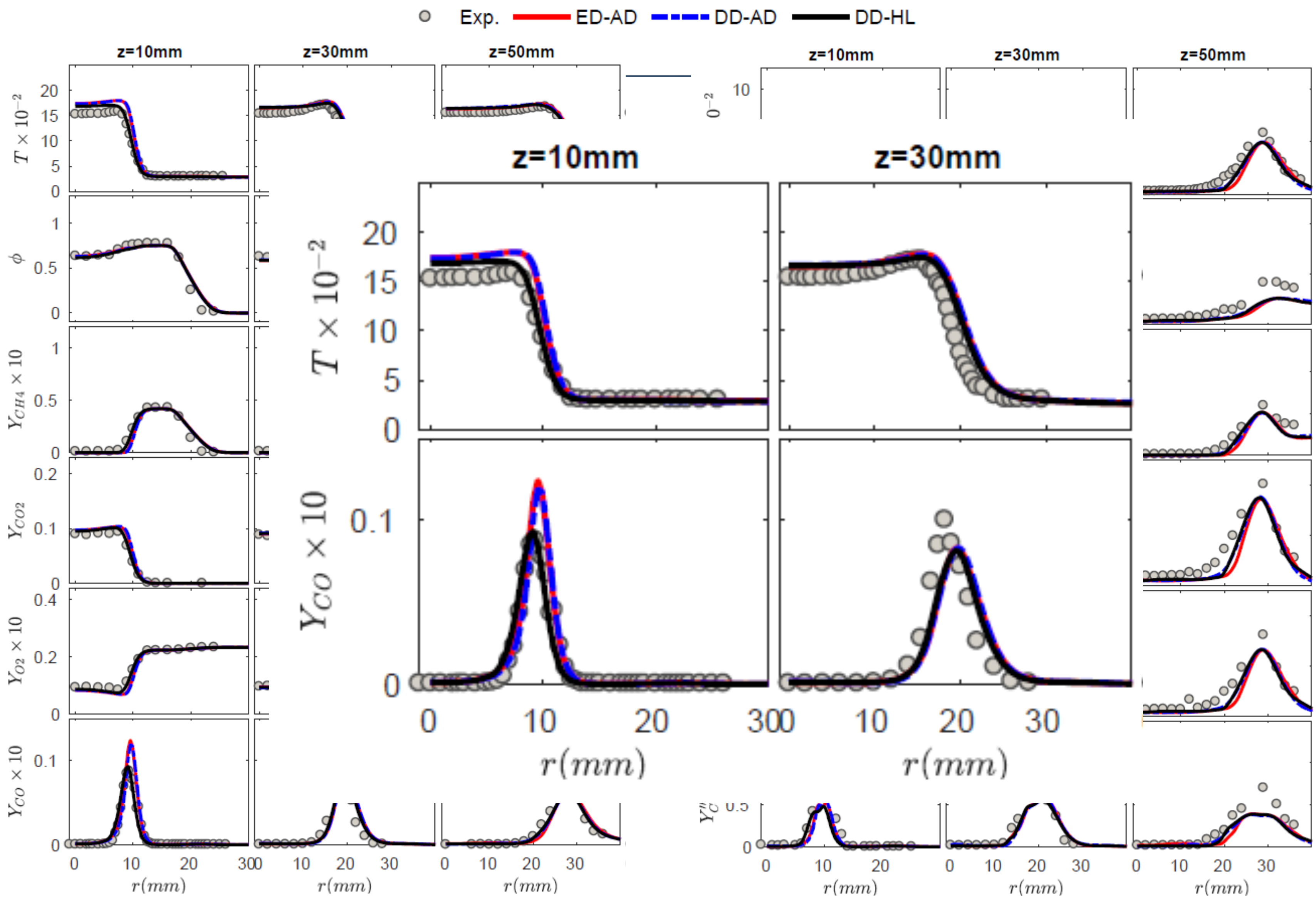
Model	Differential Diffusion	Heat Lose Effects
ED-AD	-	-
DD-AD		-
DD-HL		

[1] - Sweeney et al., Combust. Flame, 2012 . [2] - Sweeney et al., Combust. Flame, 2012.
[3] - Zhou et al., Combust. Flame, 2012.

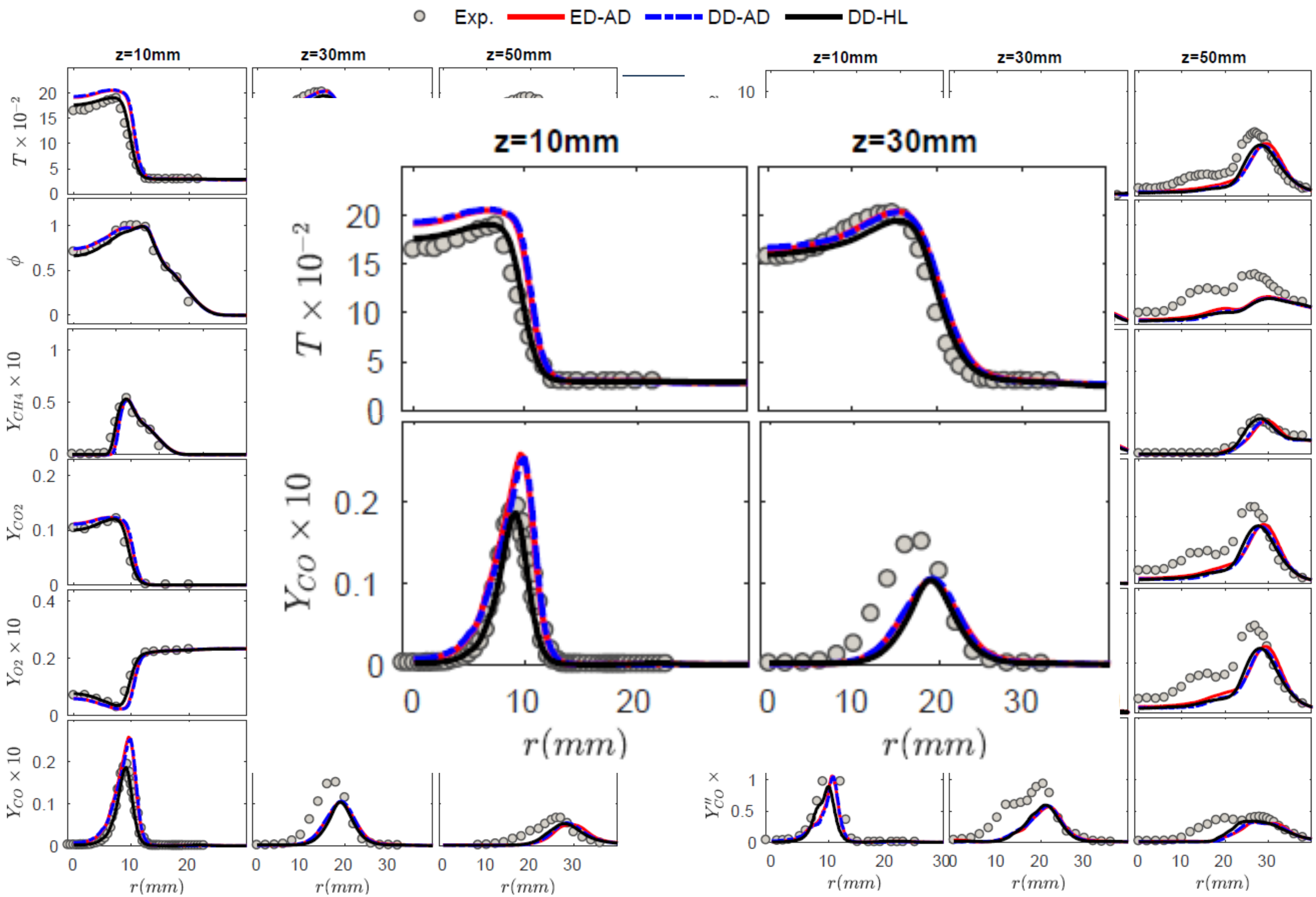
Mean Flow Fields



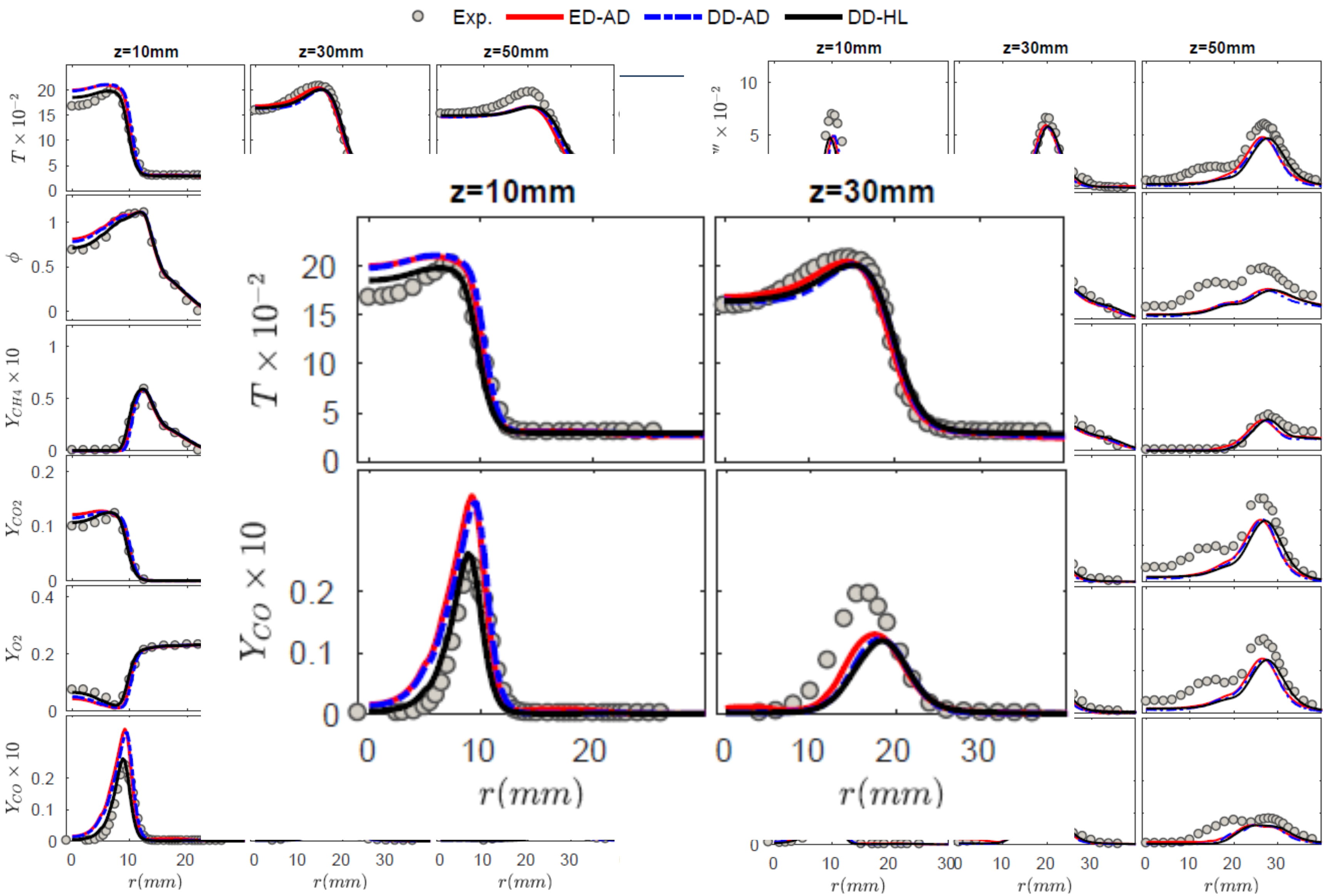
Mean and RMS: Premixed Flame – SwB3



Mean and RMS: Moderately Stratified– SwB7

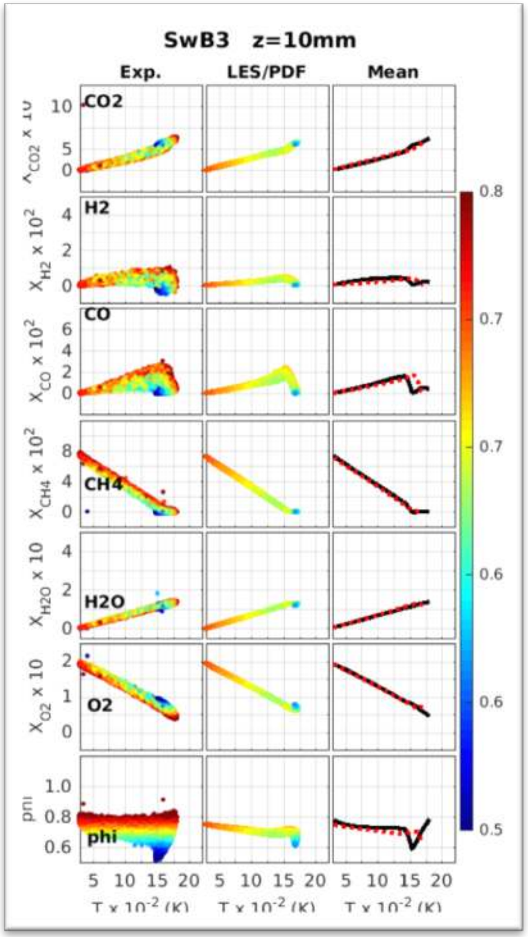


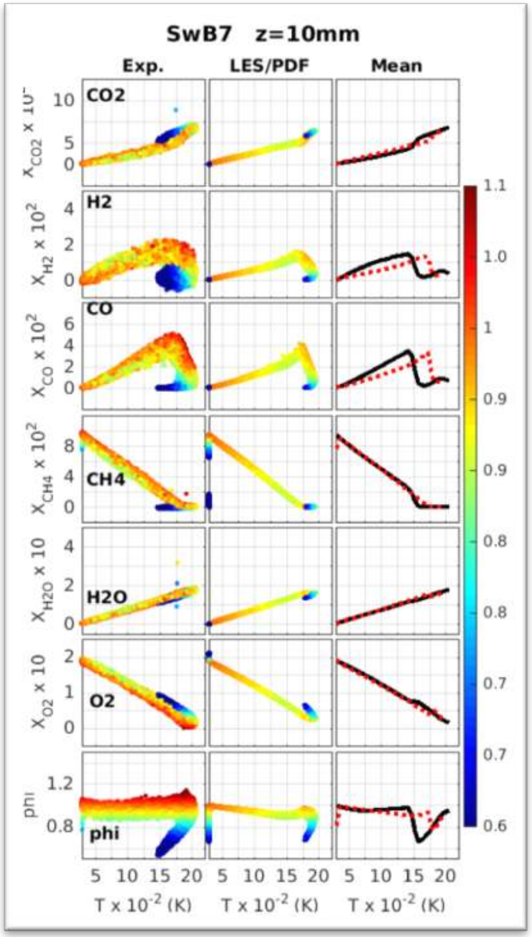
Mean and RMS: Highly Stratified– SwB11

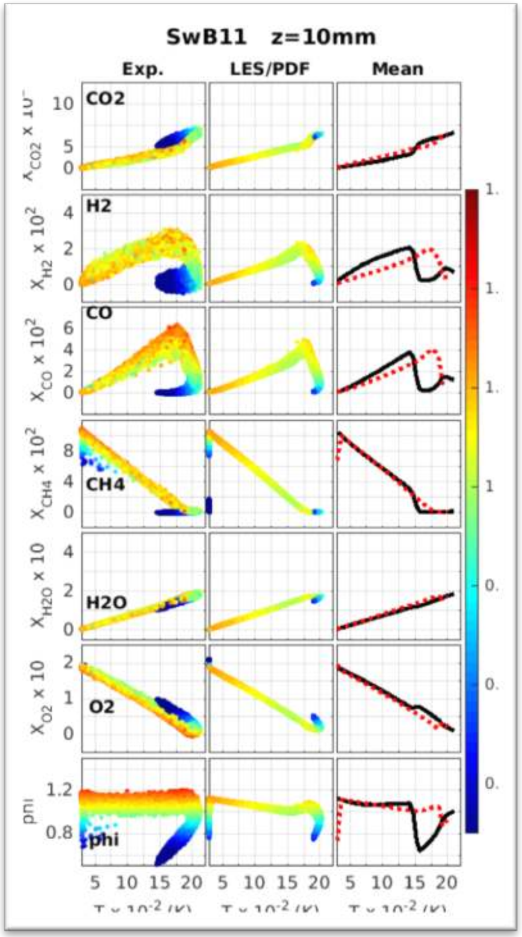


Scatter Plots: Conditional Means

Premixed Flame | Moderately Stratified Flame | Highly Stratified Flame







Conclusions

- The PDF method has a unique advantage of treating arbitrarily non-linear chemical reactions exactly
- The LES/PDF method combines advantages of LES and PDF while avoiding their deficiencies when used alone
- The hybrid LES/PDF simulator developed in OpenFOAM flatform has been shown to perform very well
- The method is designed to work on structured, block-structured and unstructured grids
- The method is found to be very successful in simulating challenging test cases of Cambridge/Sandia non-swirling and swirling stratified flames
- The method can be used as a design tool in actual combustor simulations

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  - The Scientific and Technical Research Council of Turkey (TUBITAK) (111M067, 214M309)
  - The Turkish Academy of Sciences (TUBA)
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  - Prof. Xinyu Zhao (University of Connecticut)
  - Dr. Hasret Turkeri (TEI)

Thank you!