LES OF A STRATIFIED TURBULENT BURNER WITH A THICKENED FLAME MODEL COUPLED TO ADAPTIVE MESH REFINEMENT AND DETAILED CHEMISTRY

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INTRODUCTION

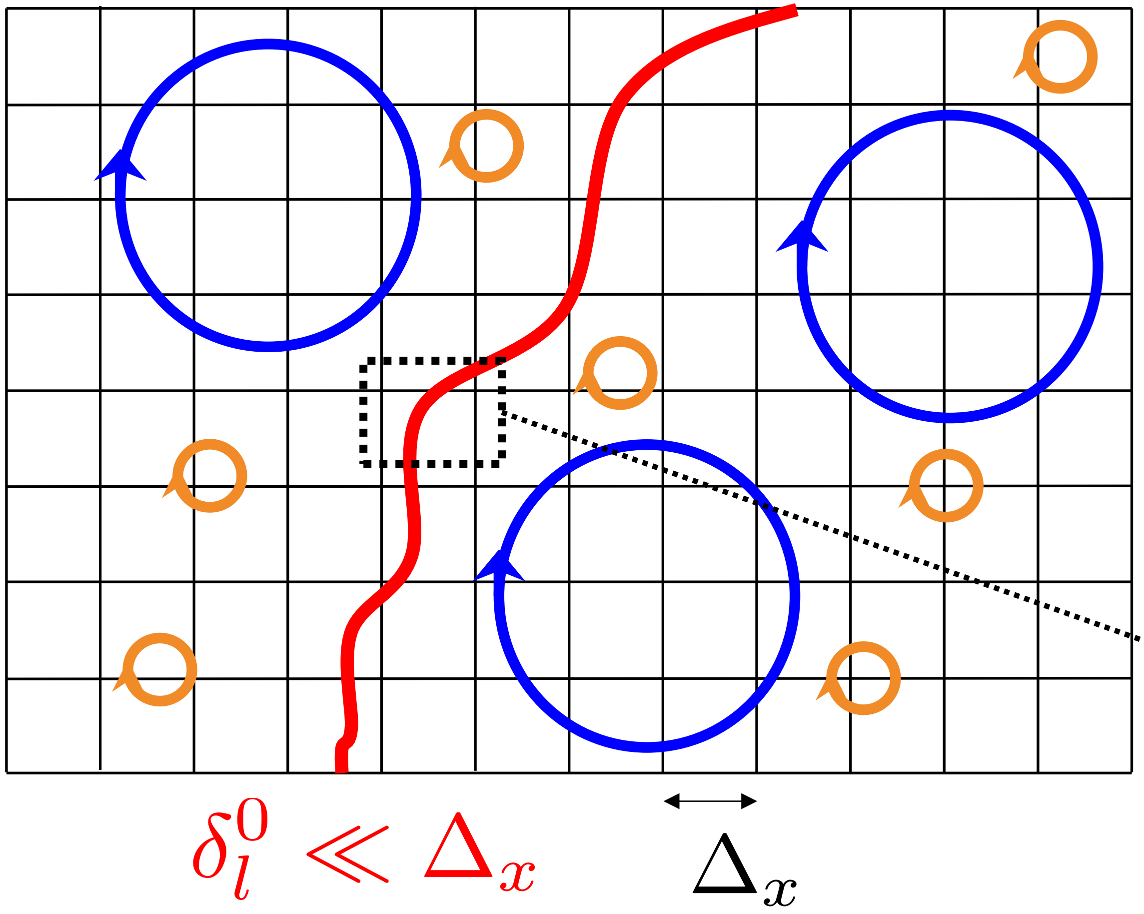
- Regulation on pollutants emissions become stricter
  => Need for highly accurate numerical tools to design systems

- Large-Eddy Simulation (LES) routinely used in the industry

- New technologies with low emissions based on **lean premixed** and **stratified** combustion regimes

MODELING ISSUES IN PREMIXED/STRATIFIED COMBUSTION

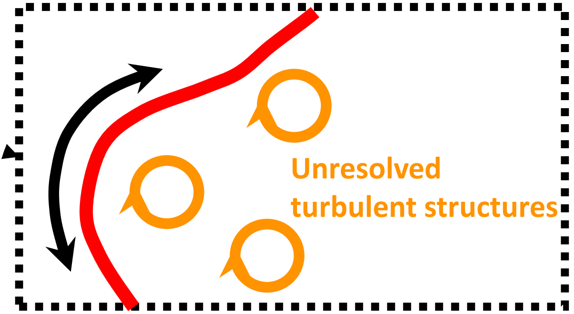
Large-Eddy Simulation (LES): Large resolved scales + small modelled scales



(Typically 0.5 to a few mm)

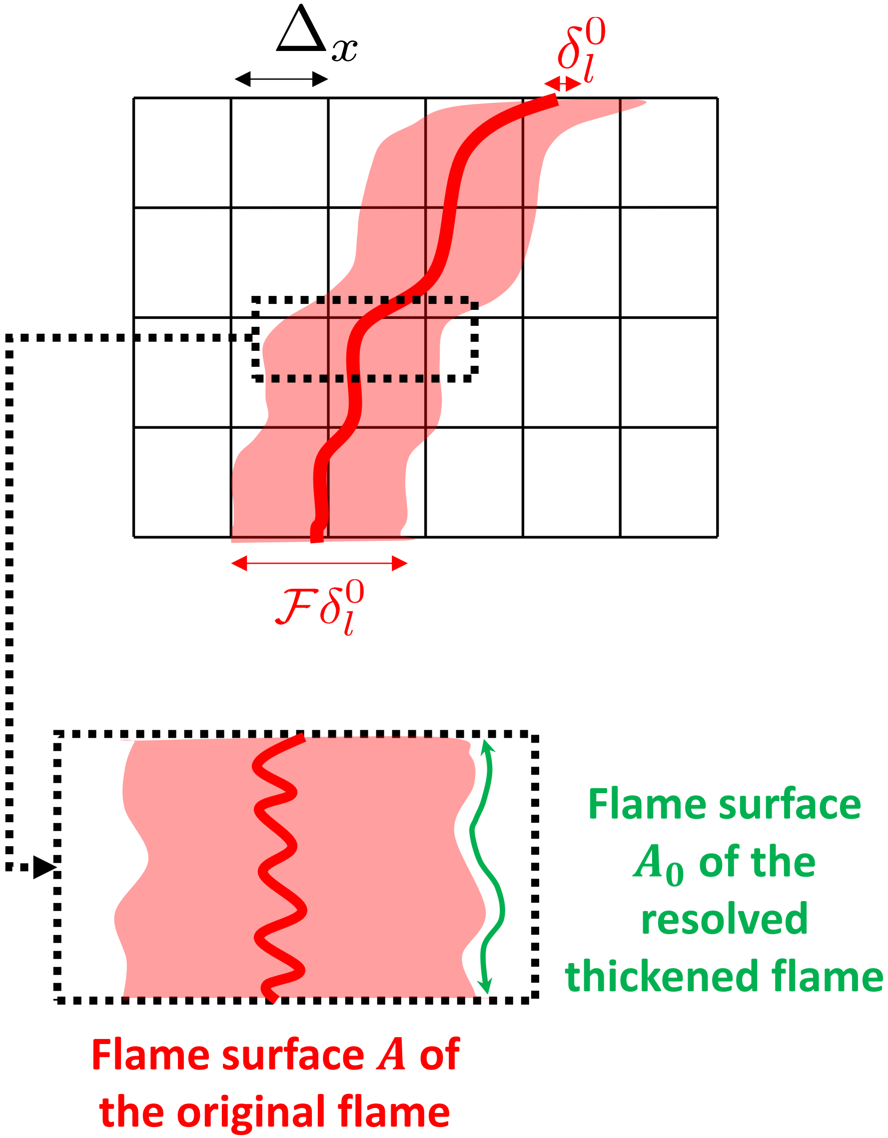
ISSUE 1: The flame structure is not resolved on the LES grid as the LES grid size is typically larger than the flame.

ISSUE 2: Interactions between unresolved turbulent structures and the flame front have to be modeled.



THICKENED FLAME MODEL (TFM)

SUSTAINABLE MOBILITY



- The flame front is artificially thickened to ensure sufficient resolution

$$\mathcal{F} = \max\left(\frac{n_{res}\Delta_x}{\delta_l^0}, 1\right)$$

- Subgrid scale (SGS) interactions described by a wrinkling factor:

$$\Xi_\Delta = \frac{A}{A_0}$$

- Turbulent flame speed propagation:

$$S_T = \Xi_\Delta S_l^0$$

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ISSUE

- Performance of the TFM model decreases when the mesh size increases (less flame/turbulence interactions resolved; more is modelled)
- LES is expensive => mesh resolution is limited
- Opportunity: Adaptive Mesh Refinement (AMR)
  - **Idea:** Refine the mesh only where necessary and hence reduce computational costs

OBJECTIVE: couple TFM and AMR to propose a model for highly accurate simulation of gas turbines at low computational cost

AGENDA

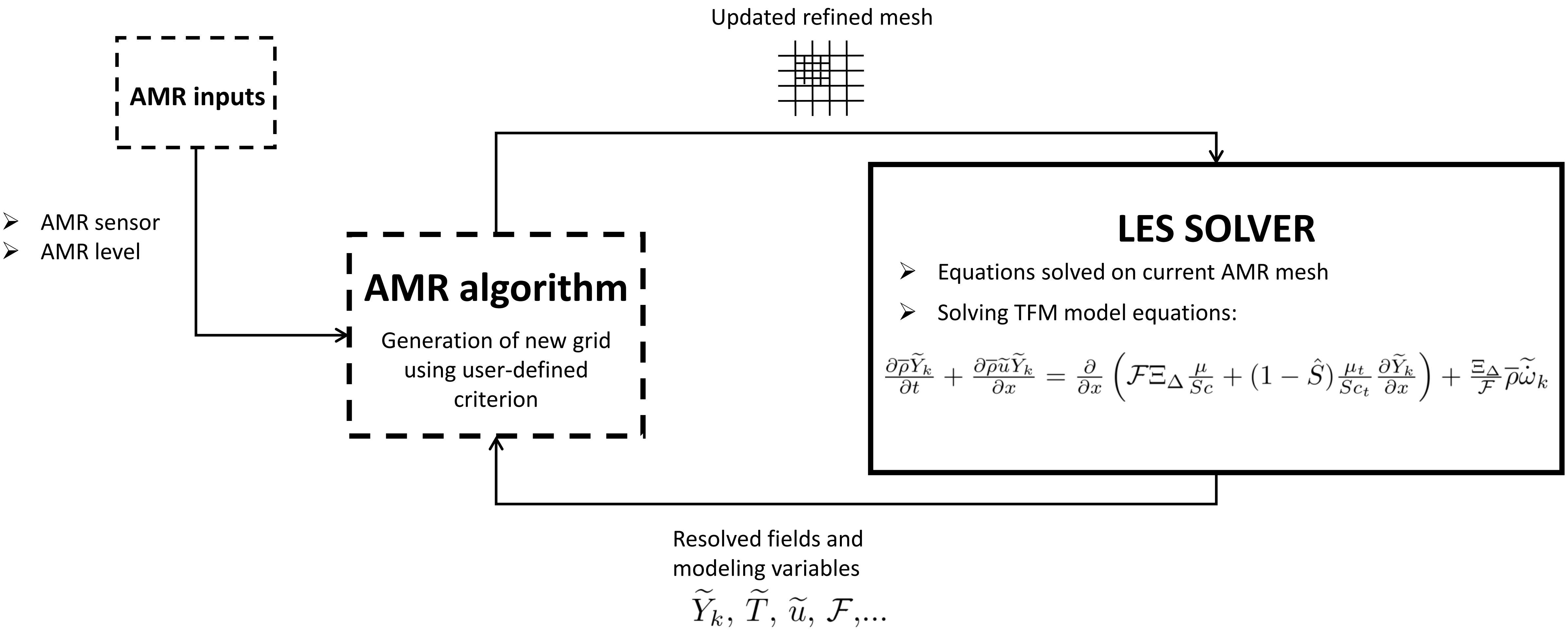
I. TFM-AMR model: coupling Thickened Flame Model with Adaptive Mesh Refinement

II. Validation of TFM-AMR on planar laminar flames

III. Simulation of the Cambridge stratified burner

IV. Conclusion

ADAPTIVE MESH REFINEMENT: PRINCIPLE



Updated refined mesh

AMR inputs

- AMR sensor
- AMR level

AMR algorithm

Generation of new grid using user-defined criterion

LES SOLVER

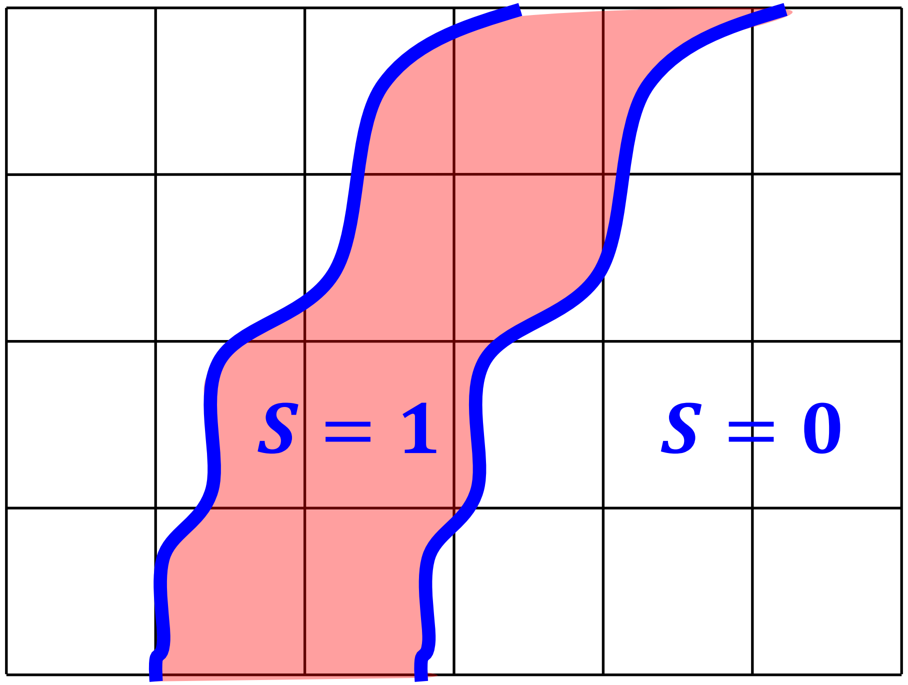
- Equations solved on current AMR mesh
- Solving TFM model equations:

$$\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}\widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x}\left(\mathcal{F}\Xi_\Delta \frac{\mu}{Sc} + (1-\hat{S})\frac{\mu_t}{Sc_t}\frac{\partial \widetilde{Y}_k}{\partial x}\right) + \frac{\Xi_\Delta}{\mathcal{F}}\overline{\rho}\widetilde{\dot{\omega}}_k$$

Resolved fields and modeling variables

$$\widetilde{Y}_k,\ \widetilde{T},\ \widetilde{u},\ \mathcal{F},\dots$$

TFM-AMR MODEL: AMR SENSOR DEFINITION



Dynamic TFM modeling framework: We only thicken in the flame

=> Definition of a flame sensor S

Redefinition of the thickening factor:

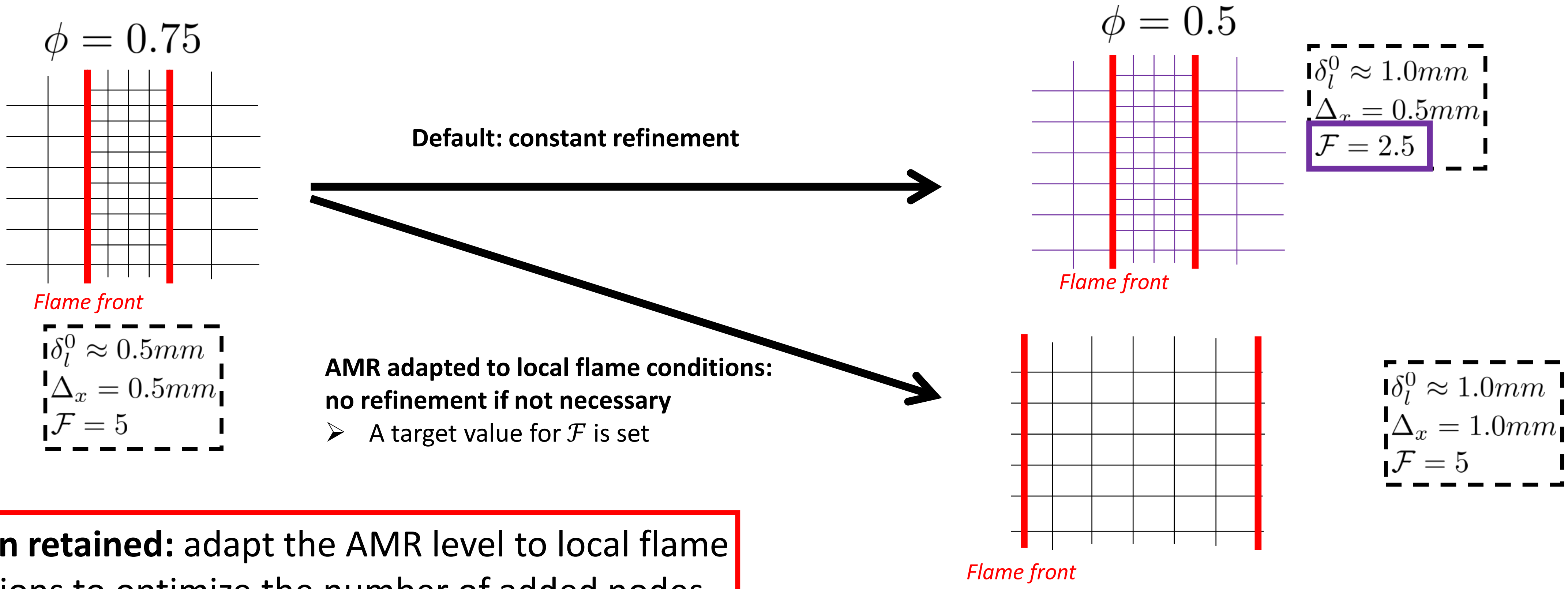
$$\mathcal{F} = \mathcal{F}_{max} + (S-1)\mathcal{F}_{max}$$

AMR is activated when $S > 0$ (equivalently: $\mathcal{F} > 1$)

TFM-AMR MODEL: AMR LEVEL DEFINITION

- AMR mesh size: $\Delta_x = \Delta_x^{Base} / 2^{n_{AMR}}$

  => Thickening factor in flame region: $\mathcal{F}_{max} = \max\left(\frac{n_{res}\Delta_x^{Base}}{2^{n_{AMR}}\delta_l^0(\phi)}, 1\right)$
- **Default strategy:** set a constant AMR refinement level when the AMR sensor is active



$\phi = 0.75$

Flame front

$\delta_l^0 \approx 0.5mm$
$\Delta_x = 0.5mm$
$\mathcal{F} = 5$

Default: constant refinement

$\phi = 0.5$

Flame front

$\delta_l^0 \approx 1.0mm$
$\Delta_x = 0.5mm$
$\mathcal{F} = 2.5$

AMR adapted to local flame conditions: no refinement if not necessary

- A target value for $\mathcal{F}$ is set

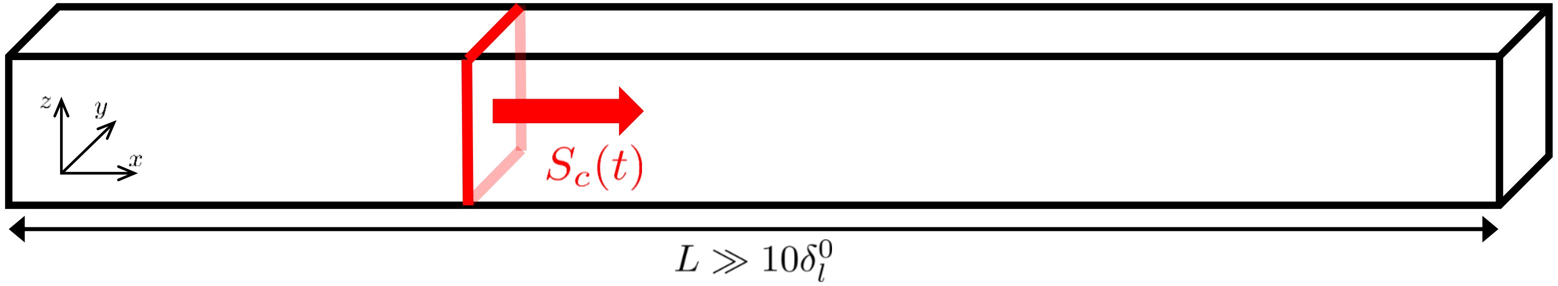
Flame front

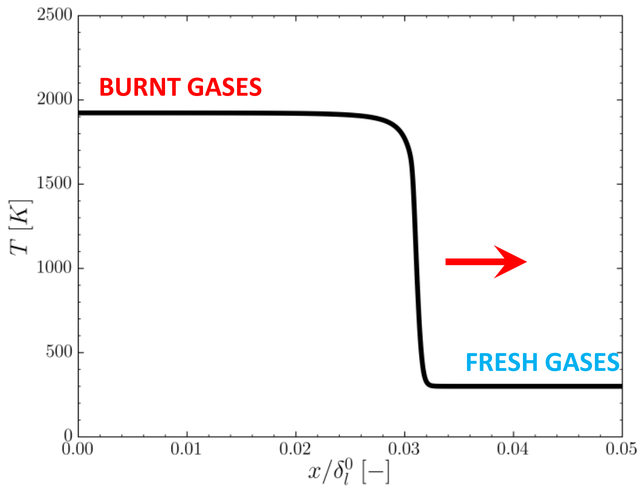
$\delta_l^0 \approx 1.0mm$
$\Delta_x = 1.0mm$
$\mathcal{F} = 5$

Solution retained: adapt the AMR level to local flame conditions to optimize the number of added nodes.

PLANAR LAMINAR FLAME SET-UP

Set-up: planar laminar flame propagation





Laminar flame propagation speed:

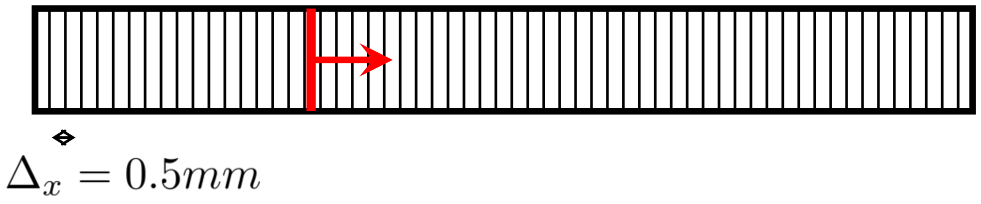
$$S_c(t) = \frac{1}{\rho_u\left(Y_{fuel}^{u} - Y_{fuel}^{b}\right)} \int_{x=-\infty}^{+\infty} \rho\dot{\omega}_{fuel}(x,t)\,dx$$

Numerical set-up:
- Solver: CONVERGE
- Equivalence ratio: $\phi = 0.75$
- 30 species skeletal mechanism for CH_4

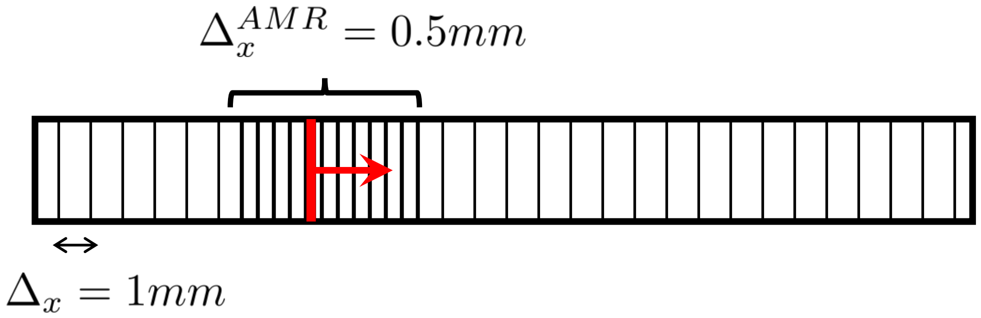
PLANAR LAMINAR FLAME SIMULATIONS

$\delta_l^0 \approx 0.5mm$

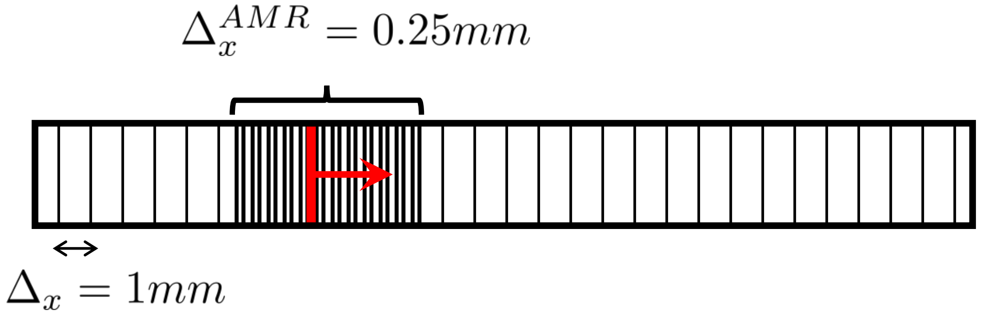
SIMULATION 1: TFM on a regular mesh



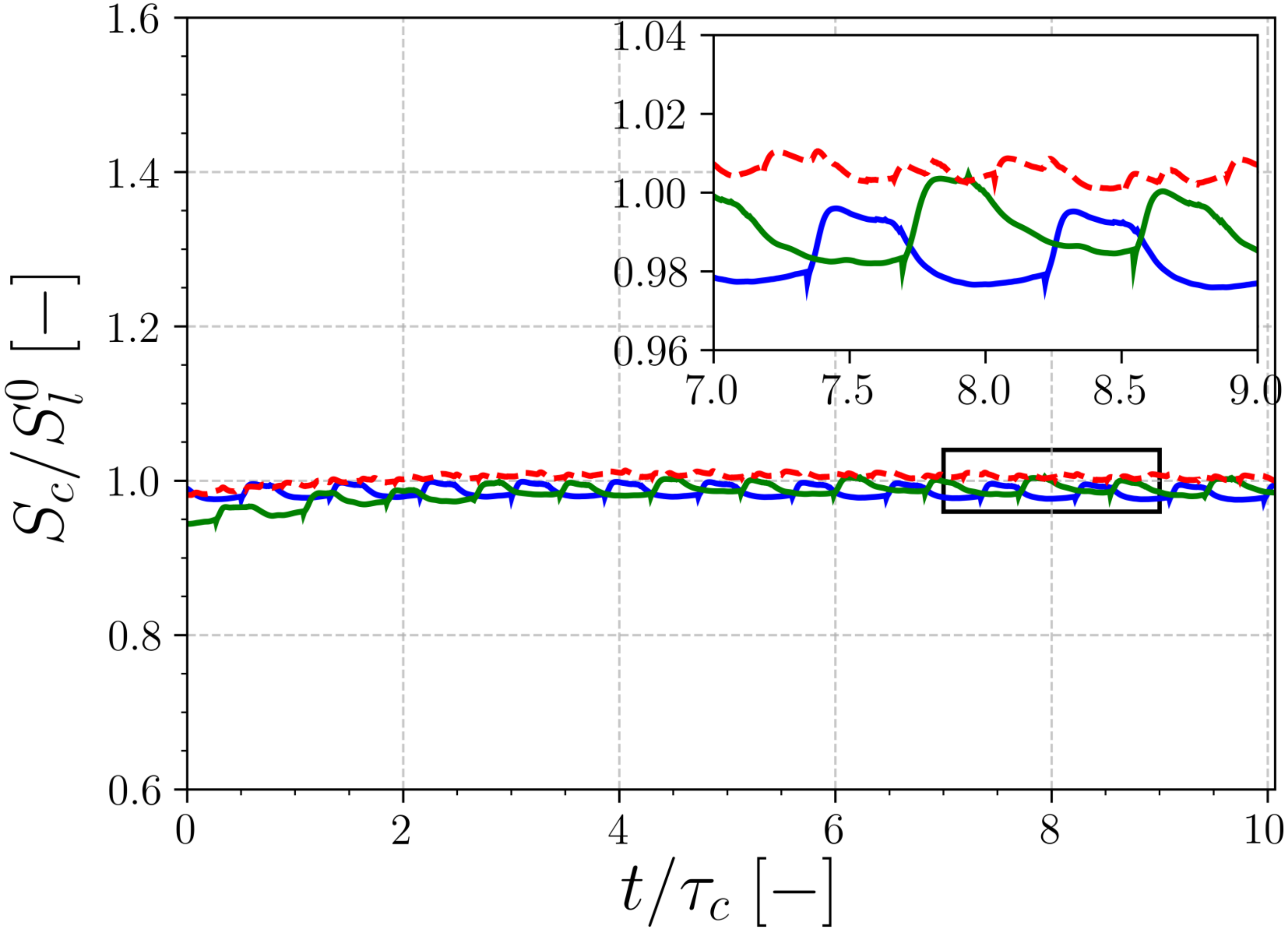
SIMULATION 2: TFM-AMR with $\mathcal{F}_{target} = 5$ on coarse mesh



SIMULATION 3: TFM-AMR with $\mathcal{F}_{target} = 2.5$ on coarse mesh



RESULTS: LAMINAR FLAME PROPAGATION

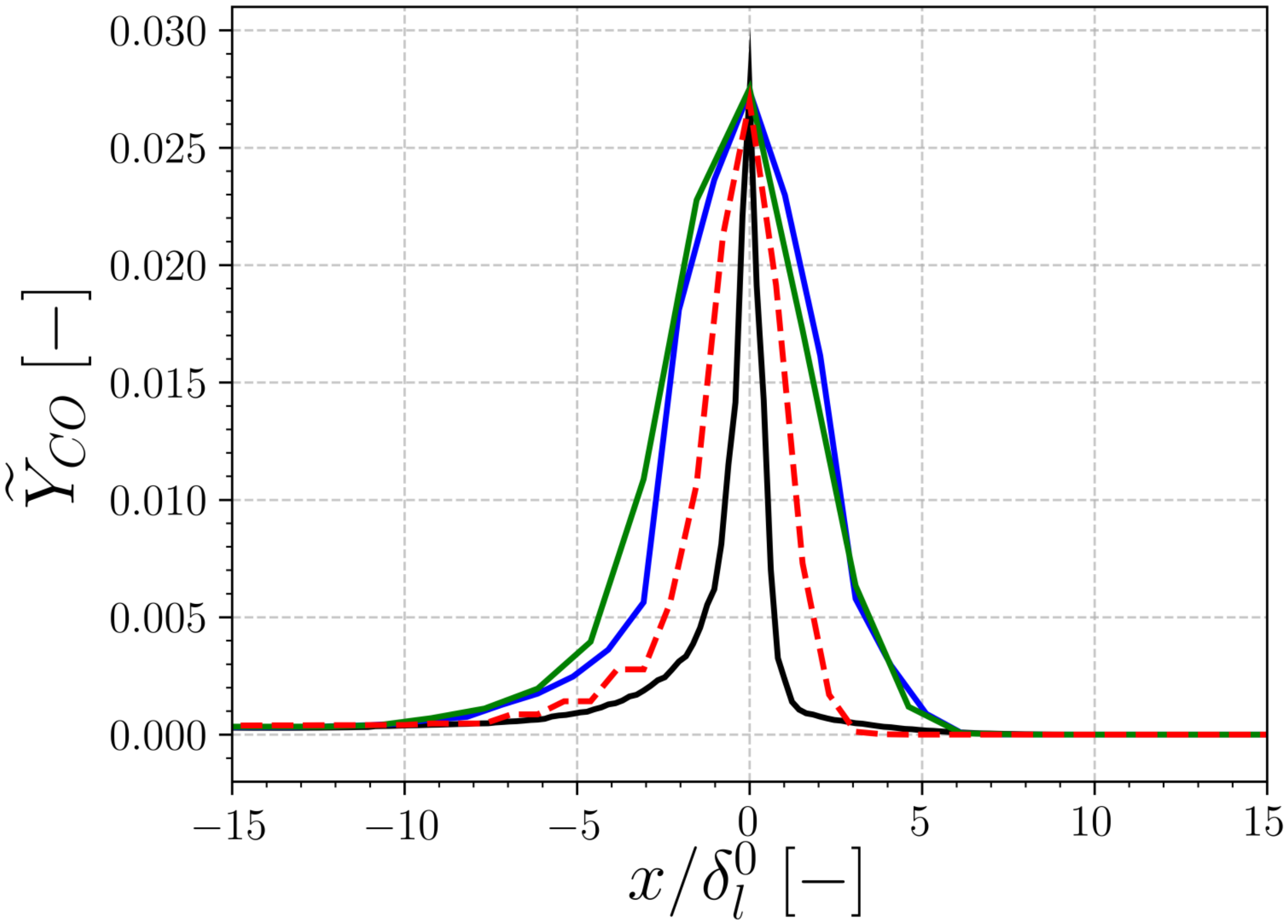


━━ : **TFM on standard mesh $(\Delta_x = 0.5\text{mm})$**

━━ : **TFM-AMR $(\mathcal{F}_{target} = 5$ => $\Delta_x = 0.5\text{mm}$ in flame)**

– – – : **TFM-AMR $(\mathcal{F}_{target} = 2.5$ => $\Delta_x = 0.25\text{mm}$ in flame)**

RESULTS: LAMINAR FLAME STRUCTURE



— : Reference laminar flame

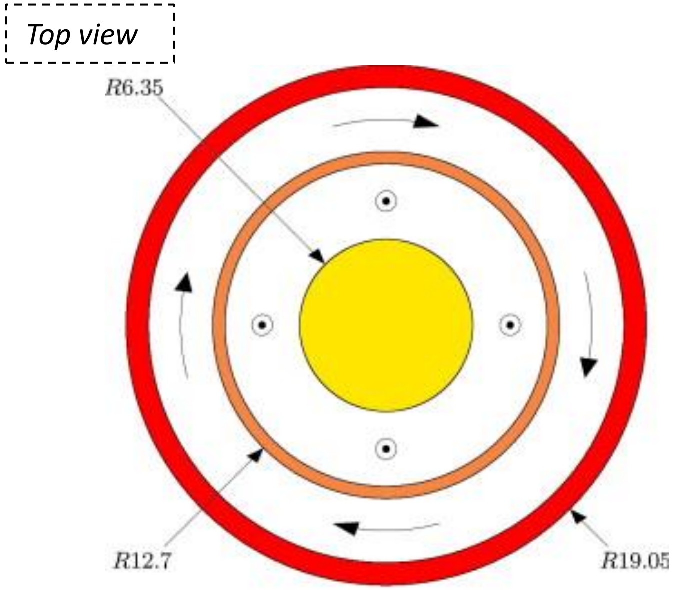
— : TFM on standard mesh ($\Delta_x = 0.5$mm)

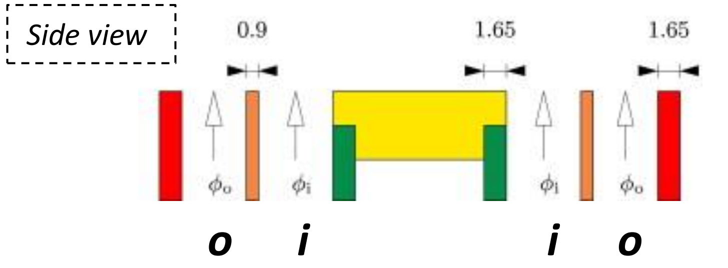
— : TFM-AMR ($\mathcal{F}_{target} = 5$ => $\Delta_x = 0.5$mm in flame)

- - - : TFM-AMR ($\mathcal{F}_{target} = 2.5$ => $\Delta_x = 0.25$mm in flame)

III. VALIDATION ON A 3-D BURNER: EXPERIMENTAL SET-UP

Cambridge SwB burner (Sweeney et al., 2012):





OPERATING CONDITIONS

Flow:

- Inner/Outer tube speeds: $U_i = 8.31$, $U_o = 18.7$
- Reynolds numbers: $Re_i = 5960$, $Re_o = 11500$

Flame:

Configuration	Inlet mixtures
SwB1 (premixed)	$\phi_i = 0.75$; $\phi_o = 0.75$
SwB5 (stratified)	$\phi_i = 1.0$; $\phi_o = 0.5$

NUMERICAL SET-UP

Solver: CONVERGE CFD SOFTWARE

Chemistry:

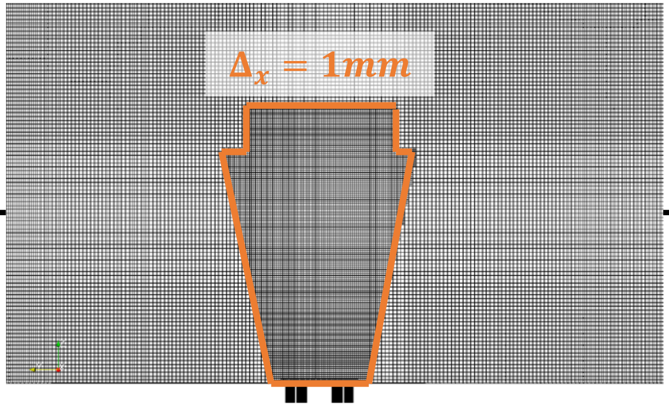
- 30 species skeletal mechanism
- SAGE chemistry solver with adaptive zoning to speed up calculations

Physical models:

- Turbulence model: SIGMA
- SGS wrinkling model : algebraic Charlette

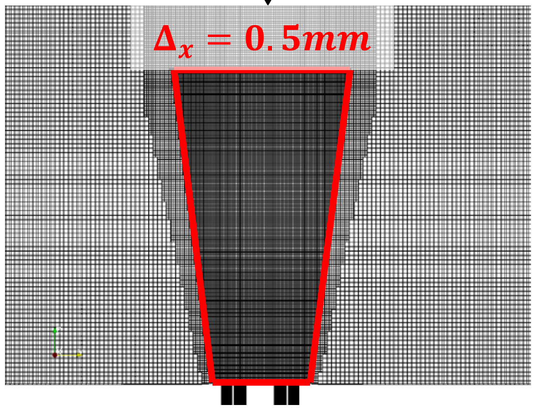
VALIDATION STRATEGY

Non-reacting flow simulation on coarse LES grid

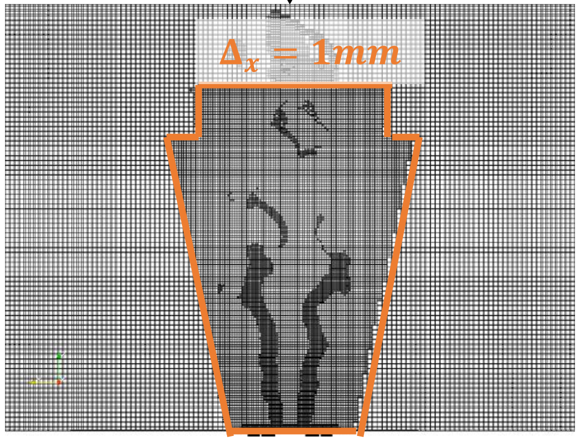


Default option (used in other CFD codes): *embedding in a large area*

New methodology: *AMR on coarse LES grid*



Comparison to validate the TFM-AMR strategy

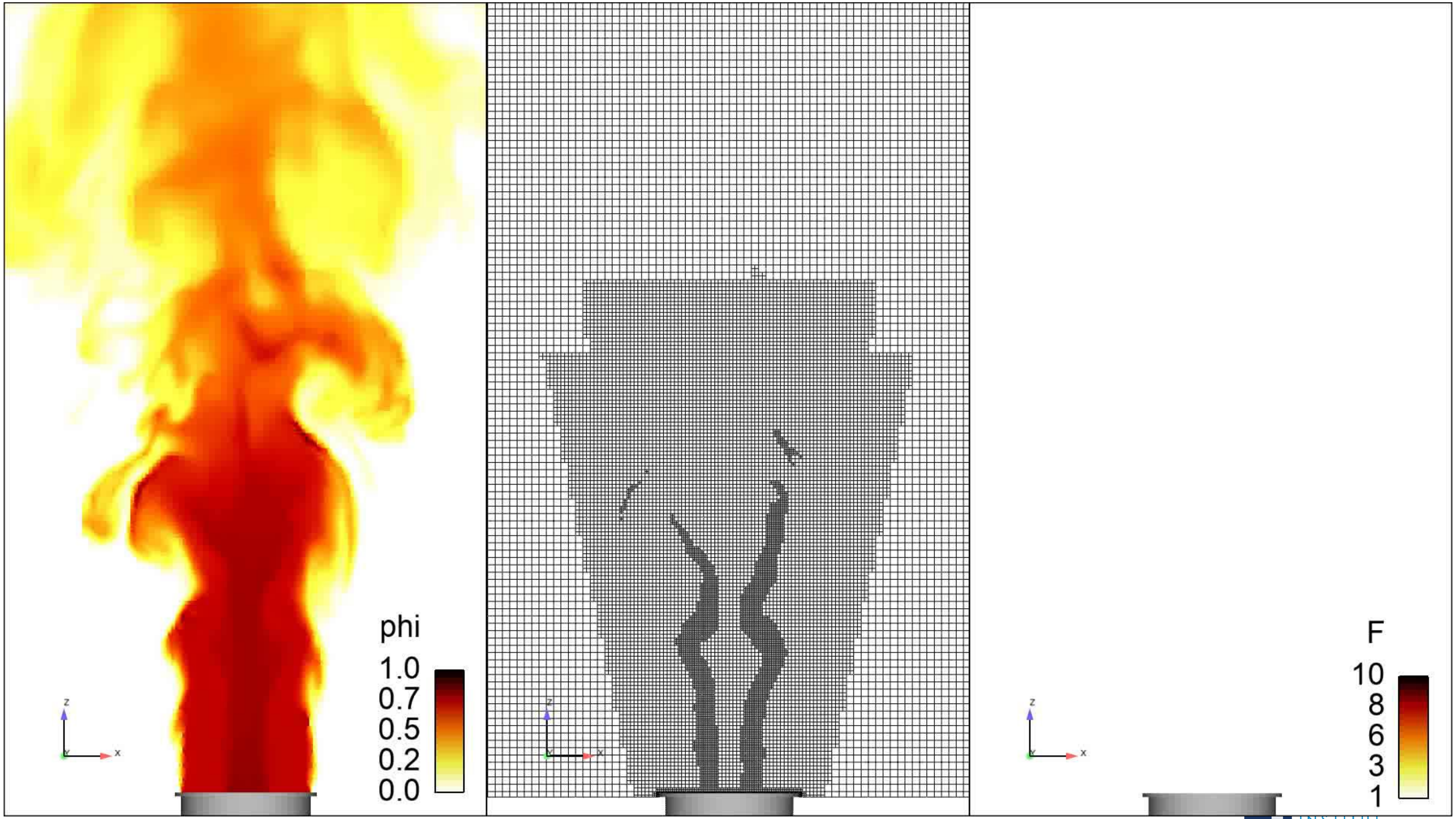


Flame simulation with TFM and embedded refined grid

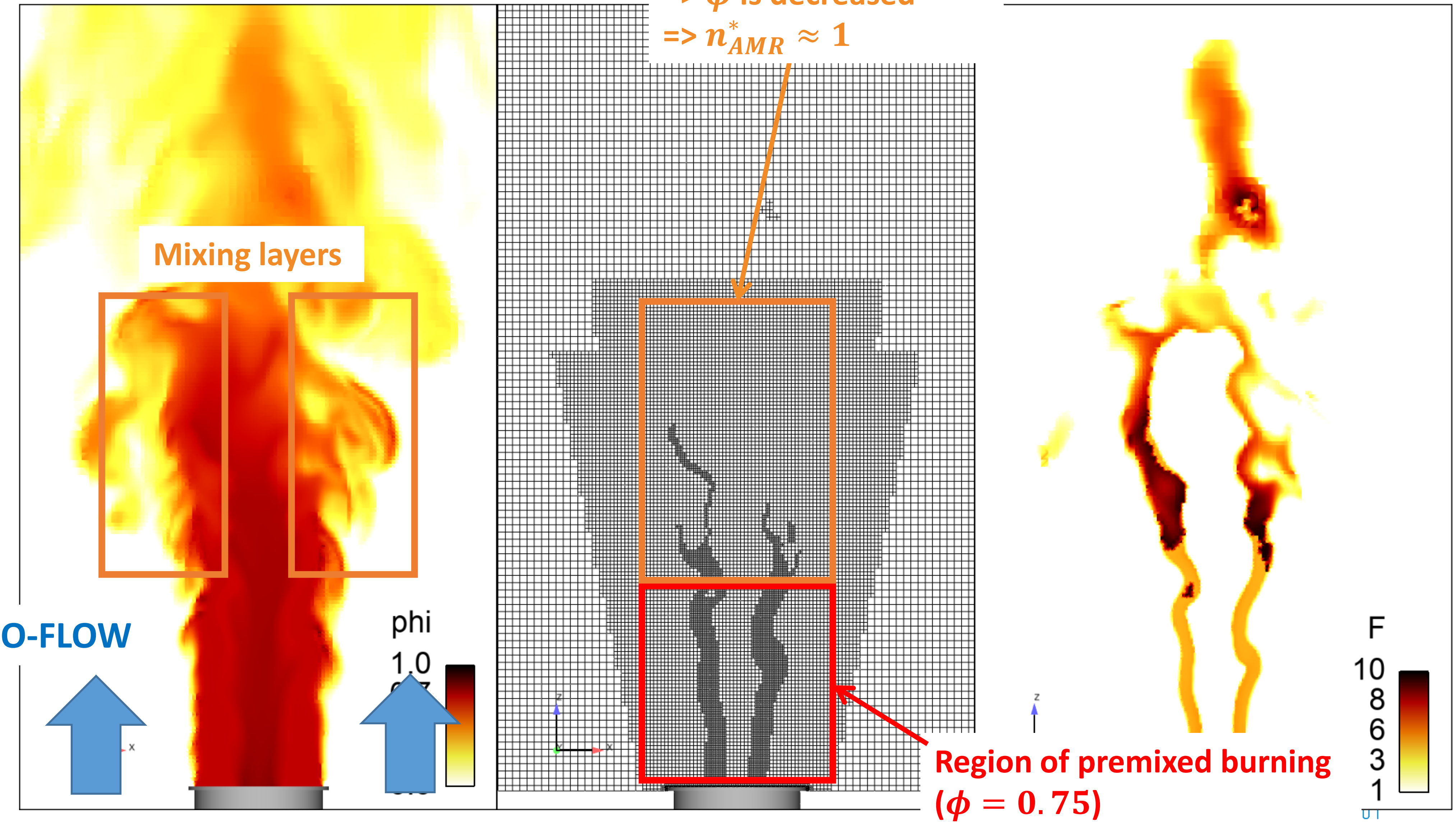
Flame simulation with TFM and AMR

$\mathcal{F}_{target} = \mathbf{5} \Rightarrow \Delta_x = 0.5mm$ for $\phi = 0.75$

TFM-AMR MODEL BEHAVIOR



TFM-AMR MODEL BEHAVIOR



Dilution by air co-flow

=> ϕ is decreased

=> $n^*_{AMR} \approx 1$

Mixing layers

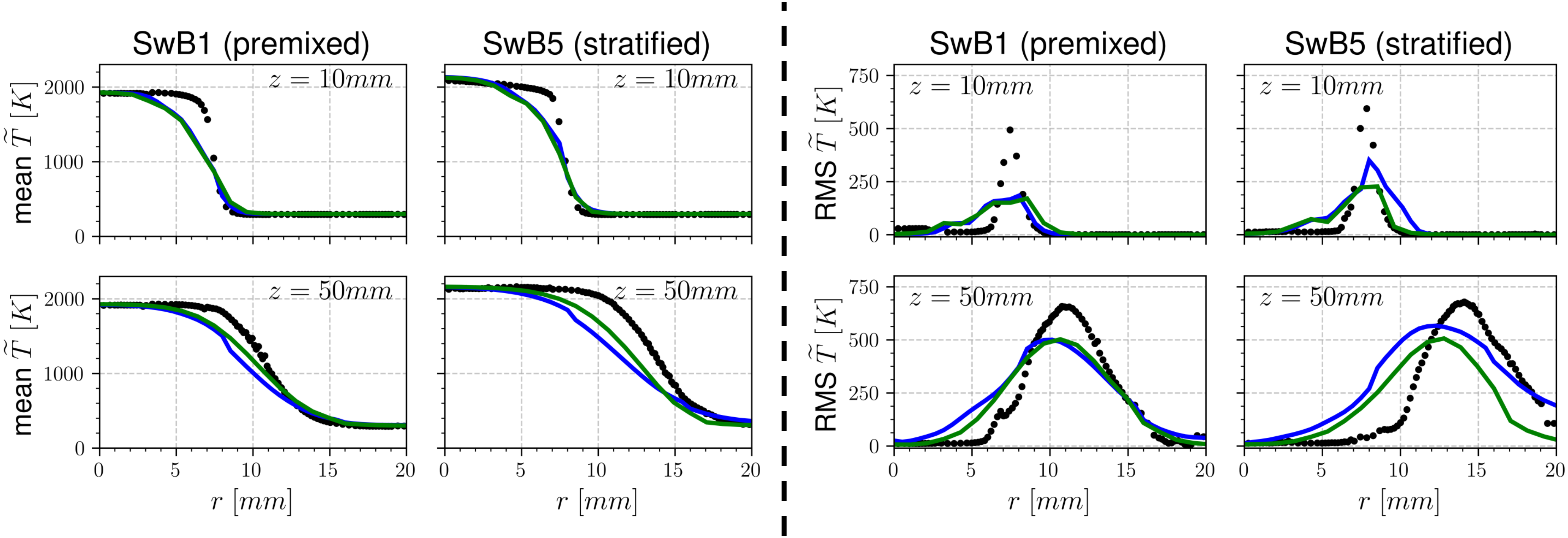
AIR CO-FLOW

Region of premixed burning

($\phi = 0.75$)

=> $n^*_{AMR} = 2$

COMPARISON WITH EXPERIMENT: TEMPERATURE



— : **Embedded TFM**

— : **TFM-AMR ($\mathcal{F}_{target} = 5$)**

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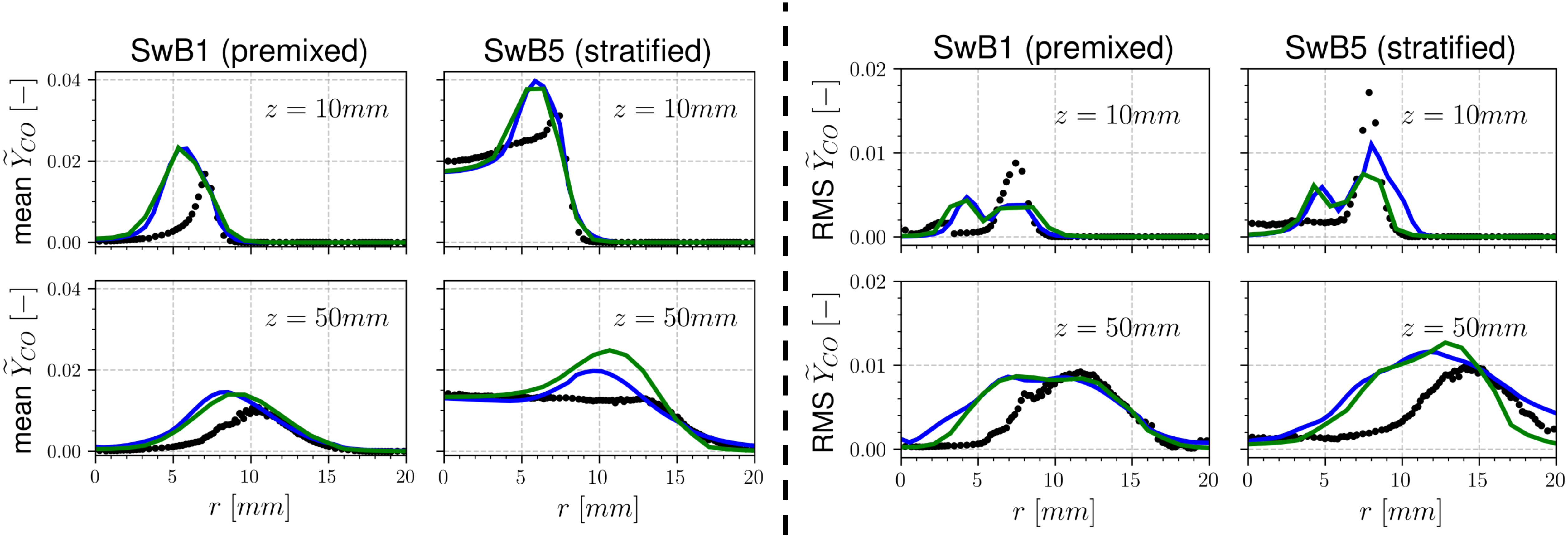
COMPARISON WITH EXPERIMENT: CARBON MONOXIDE



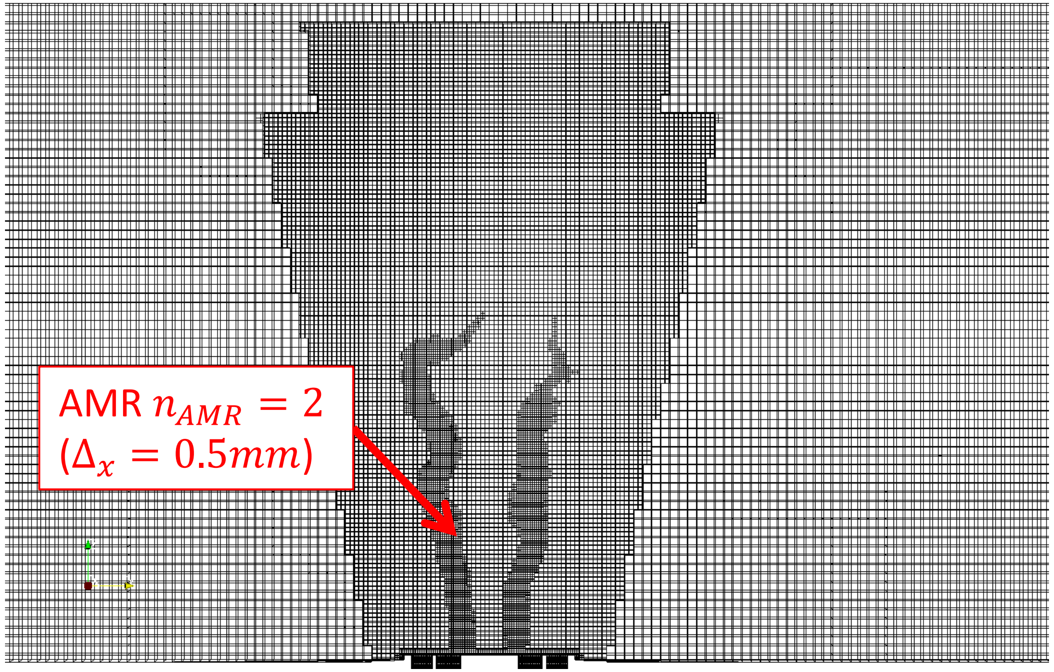
▬ : **Embedded TFM**

▬ : **TFM-AMR ($\mathcal{F}_{target} = 5$)**

AMR MESH REFINEMENT STUDY: STRATEGY

AMR refinement study:

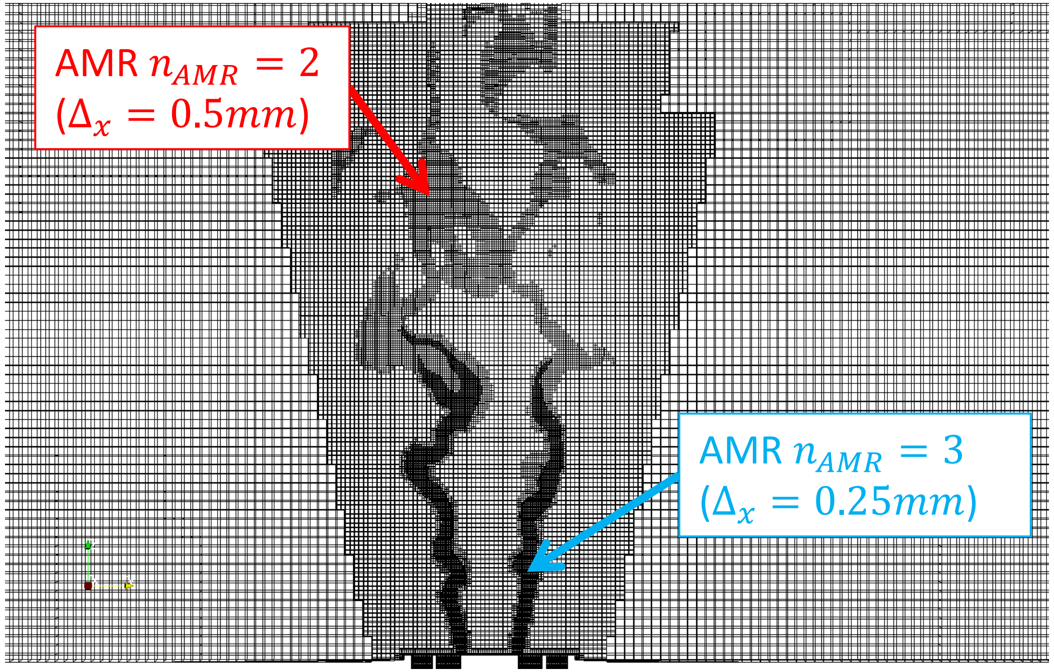
TFM-AMR with $\mathcal{F}_{target} = 5$



AMR $n_{AMR} = 2$
$(\Delta_x = 0.5mm)$

REFINEMENT

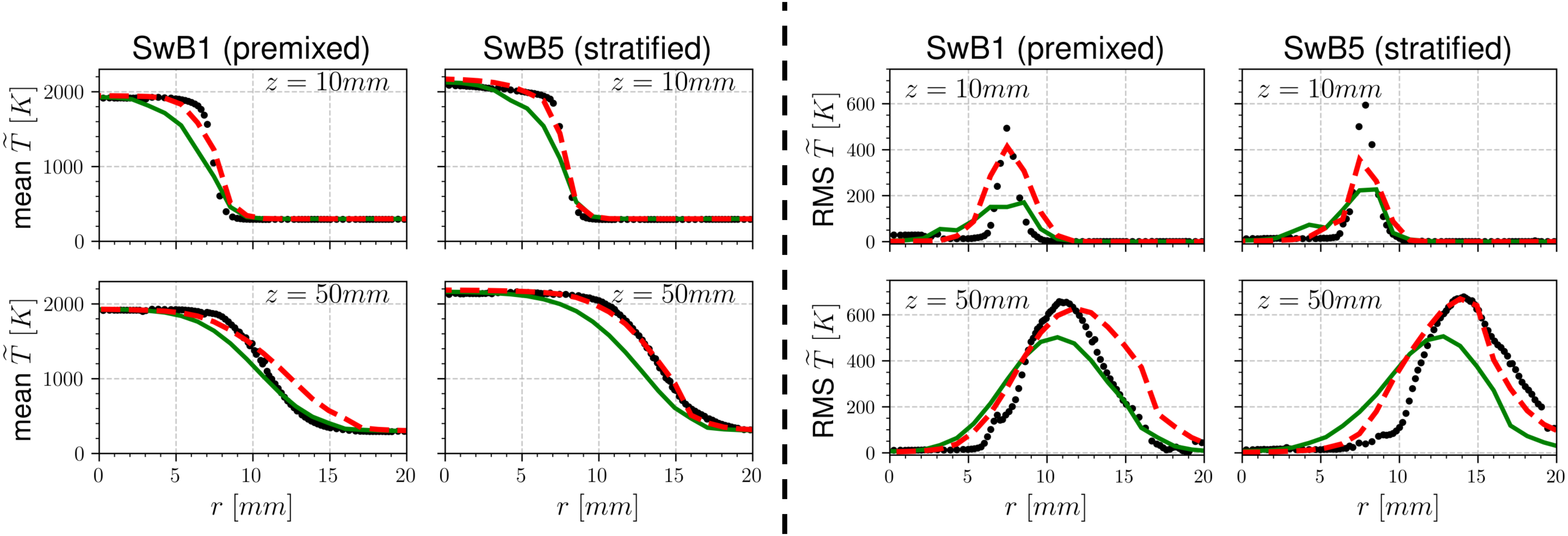
TFM-AMR with $\mathcal{F}_{target} = 2.5$



AMR $n_{AMR} = 2$
$(\Delta_x = 0.5mm)$

AMR $n_{AMR} = 3$
$(\Delta_x = 0.25mm)$

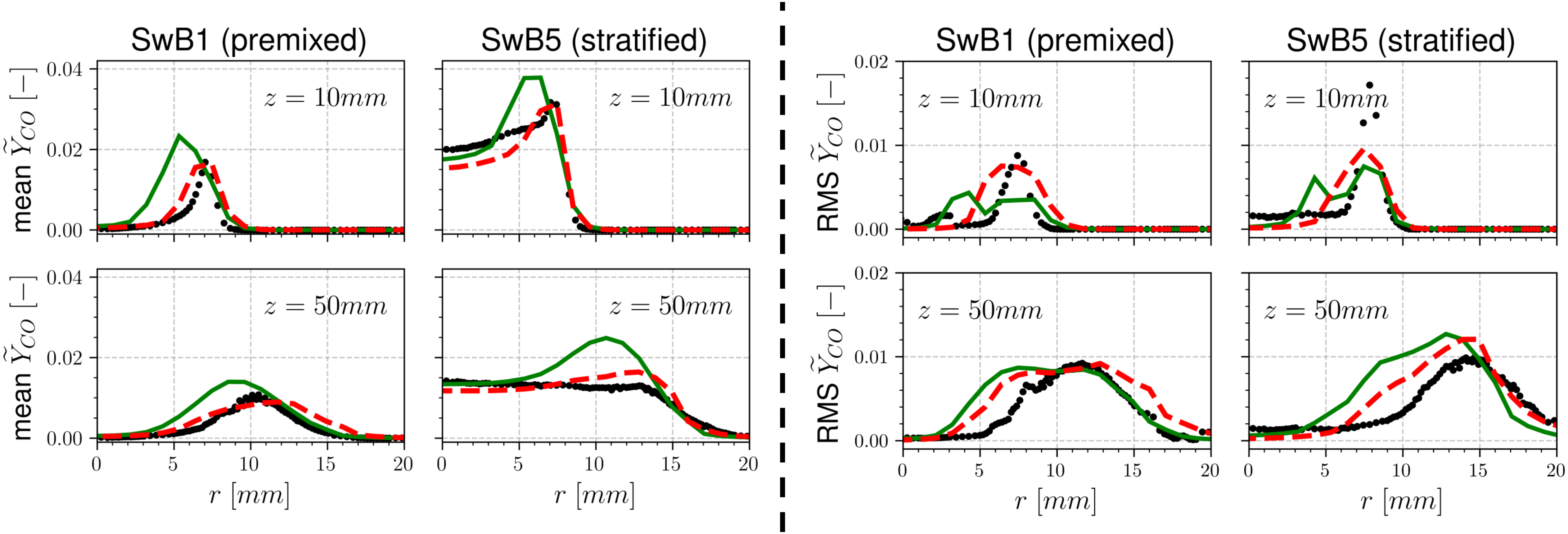
TEMPERATURE STATISTICS



— : **TFM-AMR ($\mathcal{F}_{target} = 5$)**

- - - : **TFM-AMR ($\mathcal{F}_{target} = 2.5$)**

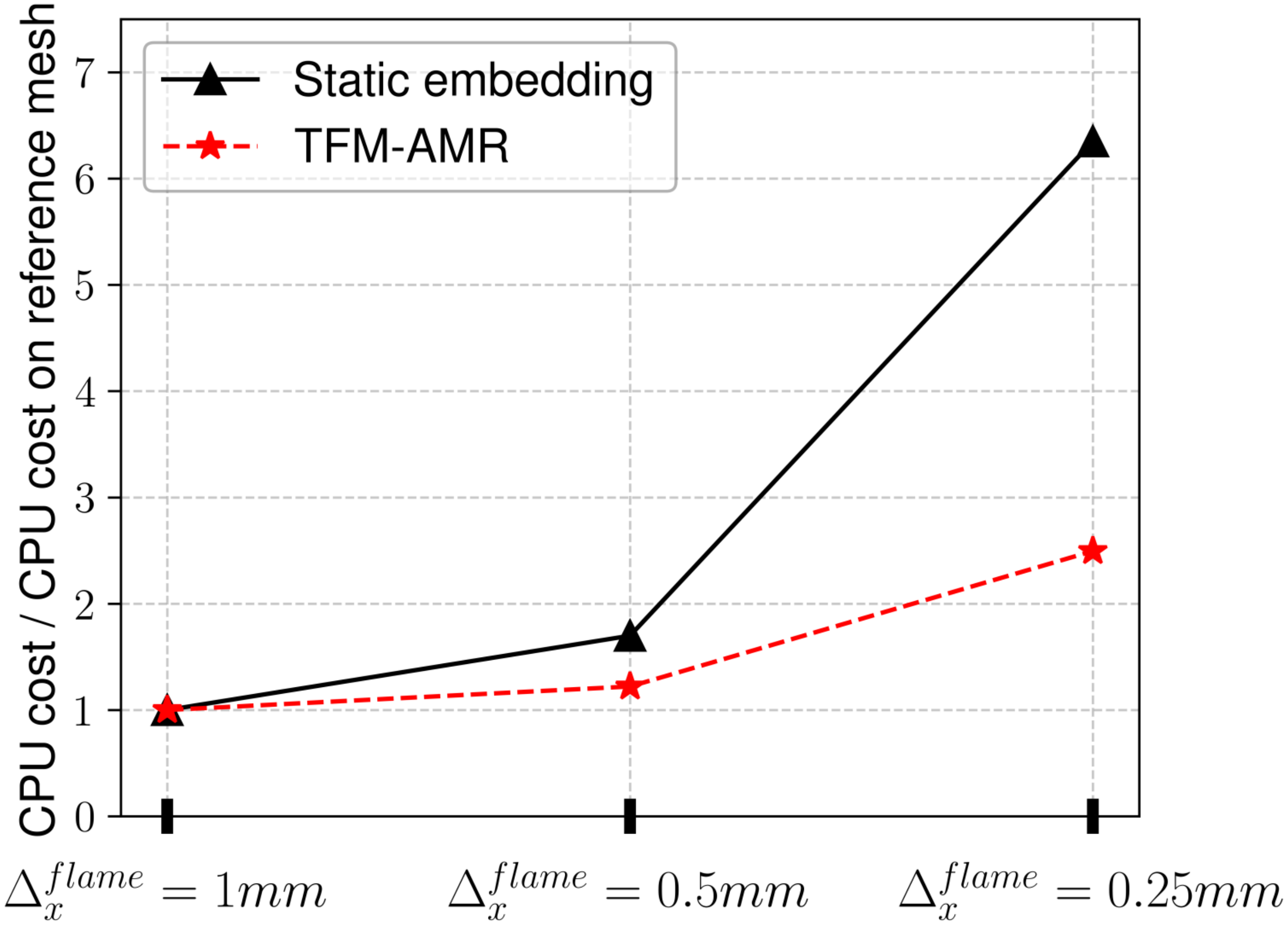
CARBON MONOXIDE STATISTICS



— : **TFM-AMR ($\mathcal{F}_{target} = 5$)**

- - - : **TFM-AMR ($\mathcal{F}_{target} = 2.5$)**

COMPUTATIONAL COSTS



CONCLUSION AND PERSPECTIVES

- A new model based on the coupling between Thickened Flame Model (TFM) and Adaptive Mesh Refinement (AMR) has been developed for premixed and stratified combustion.

- TFM-AMR model has been validated on the Cambridge swirled burner in premixed and stratified operating conditions.

- **Conclusions:**
  - TFM-AMR leads to an optimization of the flame simulation providing iso-resolution at lower computational cost compared to conventional simulations.
  - For similar costs, TFM-AMR enables to perform simulations with a better mesh resolution and hence improving predictions.

- **Perspectives:**
  - In depth study of unresolved turbulence / flame interactions when using TFM-AMR
  - Extension of TFM-AMR to spray combustion

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BACK-UP

REFERENCES

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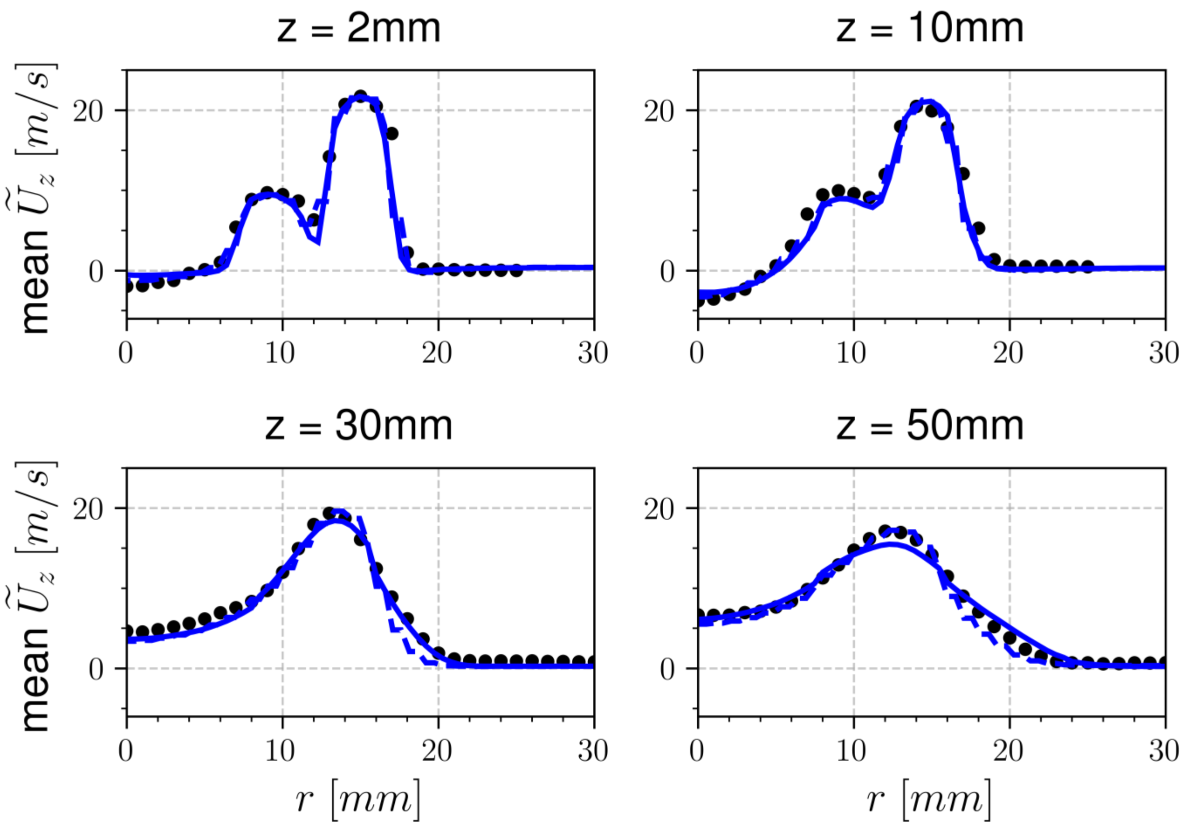
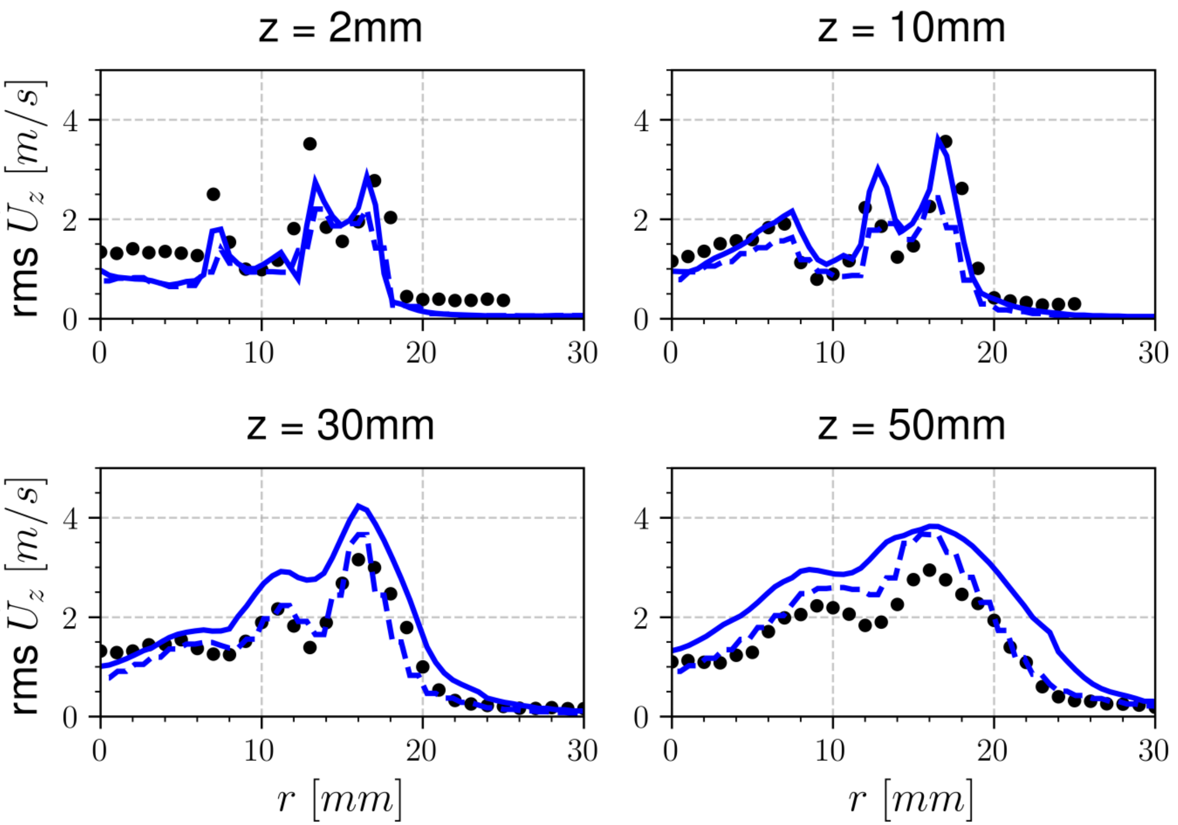
- O. Colin, F. Ducros, D. Veynante, T. Poinsot (2000), A thickened flame model for large eddy simulations of turbulent premixed combustion, Physics of Fluids, Volume 12.
- M. S. Sweeney, S. Hochgreb, M. J. Dunn, R. S. Barlow (2012), The structure of turbulent stratified and premixed methane/air flames I: Non-swirling flows, Combustion and Flame, Volume 159, Pages 2896-2911.
- P. S. Volpiani, T. Schmitt, D. Veynante (2017), Large eddy simulation of a turbulent swirling premixed flame coupling the TFLES model with a dynamic wrinkling formulation, Combustion and Flame, Volume 180, Pages 124-135.
- G. Wang, M. Boileau, D. Veynante (2011), Implementation of a dynamic thickened flame model for large eddy simulations of turbulent premixed combustion, Combustion and Flame, Volume 158.Pages 2199-2213.

RESULTS: NON-REACTING FLOW





– – – – : Simulation on coarse grid

—— : Simulation on refined grid

FLAME THICKENING

- **Thickening factor:** the flame is broadened by a factor $\mathcal{F} = \max\left(\frac{n_{res}\Delta_x}{\delta_l^0(\phi)}, 1\right)$

Where n_{res} is the number of grid points in the flame thickness

- **Scaling laws:** $\delta_l^0 \propto \sqrt{\frac{D_{th}}{\dot{\Omega}}}$ **and** $S_l^0 \propto \sqrt{D_{th}\dot{\Omega}}$

D_{th}: Heat diffusivity
$\dot{\Omega}$: Mean reaction rate

- **Modeling requirements:** $\delta_l^0 \rightarrow \mathcal{F}\delta_l^0$ and $S_l^0 \rightarrow S_l^0$
  - **Diffusion multiplied by $\mathcal{F}$ and reaction rates by $1/\mathcal{F}$**

- **Transport equation for species mass fractions:**

$$\frac{\partial \bar{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial \bar{\rho}\widetilde{u}\widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x}\left(\mathcal{F}\frac{\mu}{Sc}\frac{\partial \widetilde{Y}_k}{\partial x}\right) + \frac{1}{\mathcal{F}}\bar{\rho}\widetilde{\dot{\omega}}_k$$

SPECIES MASS FRACTIONS TRANSPORT EQUATIONS

- Final transport equation for species mass fractions (TFM model):

$$\boxed{\frac{\partial \overline{\rho}\widetilde{Y}_k}{\partial t} + \frac{\partial \overline{\rho}\widetilde{u}\widetilde{Y}_k}{\partial x} = \frac{\partial}{\partial x}\left(\mathcal{F}\Xi_\Delta \frac{\mu}{Sc} + (1-\hat{S})\frac{\mu_t}{Sc_t}\frac{\partial \widetilde{Y}_k}{\partial x}\right) + \frac{\Xi_\Delta}{\mathcal{F}}\overline{\rho}\widetilde{\dot{\omega}}_k}$$

- ✓ Resolution of the flame front thickness
- ✓ Accurate turbulent propagation speed
- ✓ Only flame front is thickened

TFM-AMR MODELING STRATEGY: AMR LEVEL COMPUTATION

- Principle:
  - Setting a target flame thickening value $\mathcal{F}_{target}$
  - Computing the theoretical AMR level n^*_{AMR} to reach the $\mathcal{F}_{target}$ value

- Relationship between n^*_{AMR} and $\mathcal{F}_{target}$:

$$\frac{\delta_l^0(\phi)\mathcal{F}_{target}}{n_{res}} = \frac{\Delta_x^{Base}}{2^{n^*_{AMR}}}$$

- Theoretical AMR level:

$$\boxed{n^*_{AMR} = \frac{1}{log(2)} log\left(\frac{n_{res}\Delta_x^{Base}}{\delta_l^0(\phi)\mathcal{F}_{target}}\right)}$$