Virtual chemistry for temperature and pollutant prediction in LES of non-adiabatic turbulent flames

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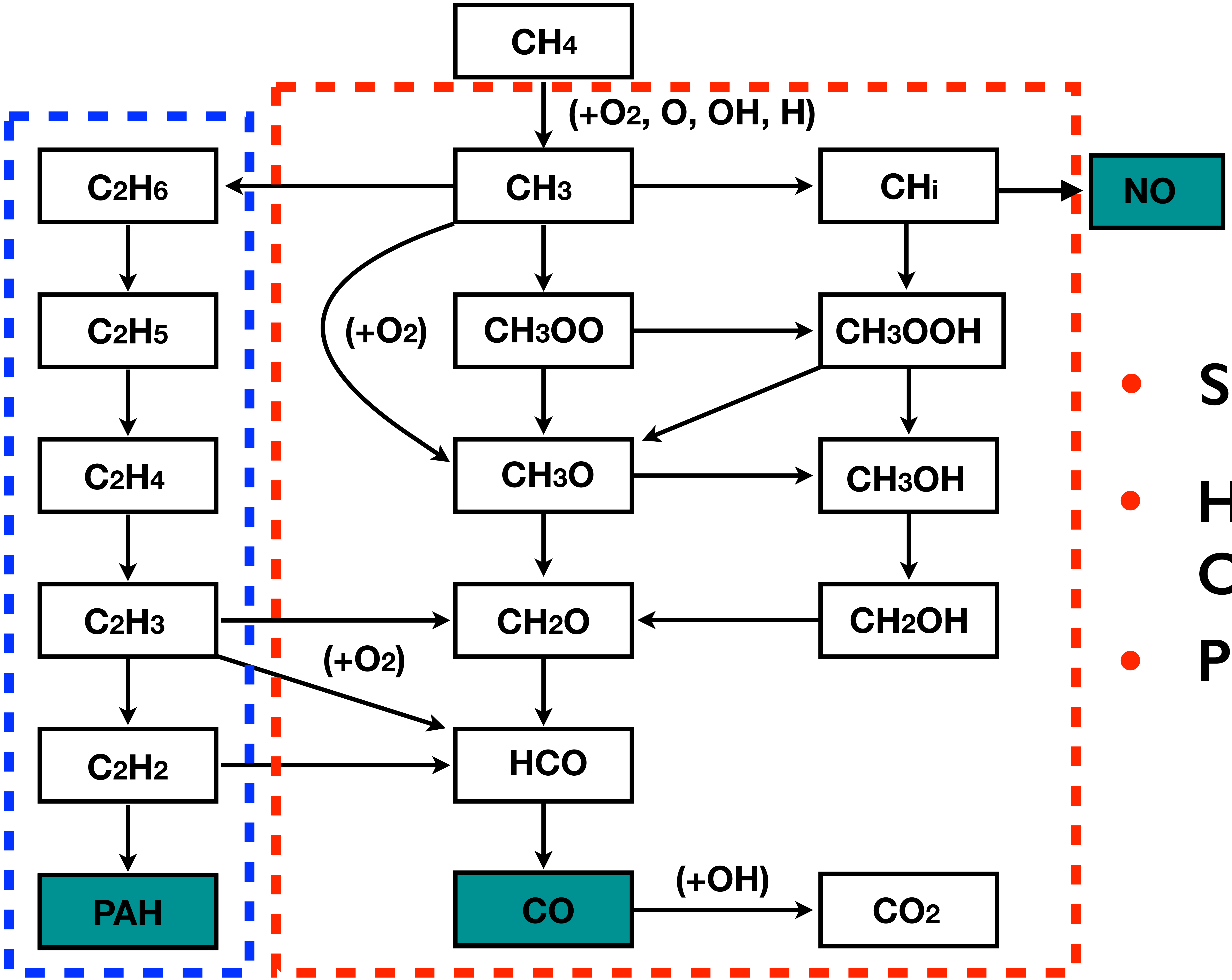
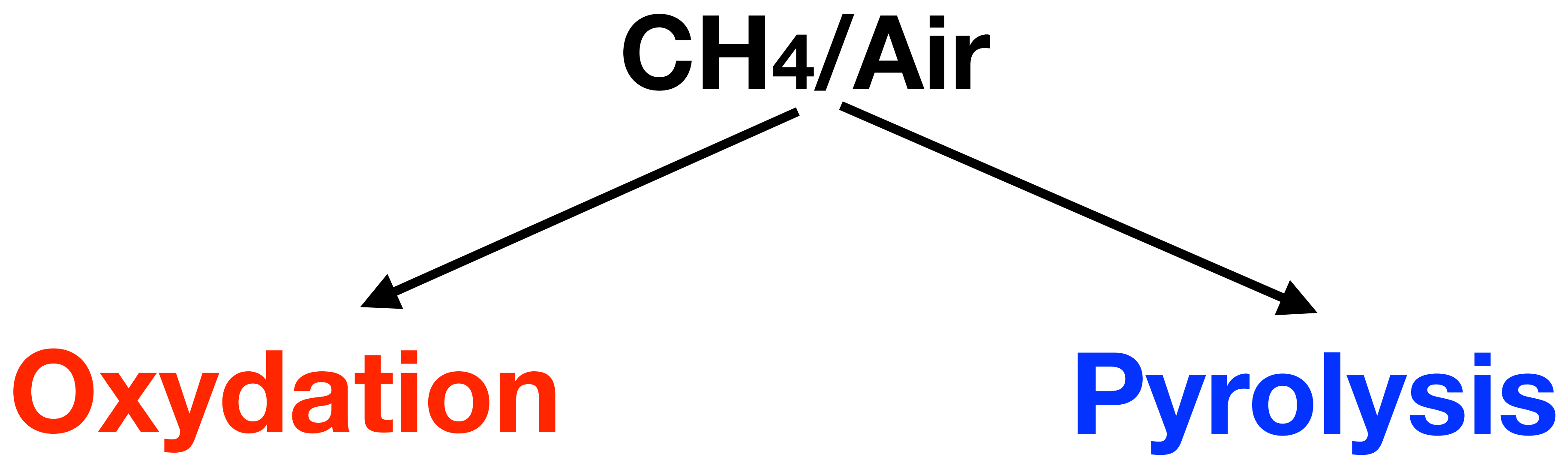
Journées conjointes Groupement de Recherche CNRS Feux - Groupement Français de Combustion

Hydrocarbon/O_2 kinetic model - pollutant formation



E. Ranzi et al. (1994)
Henry J. Curran (2018)



- Several path from $CH_4 \rightarrow CO_2$
- High / Lox temperature Oxydation
- Pollutant formation :
  - CO
  - NO
  - PAH

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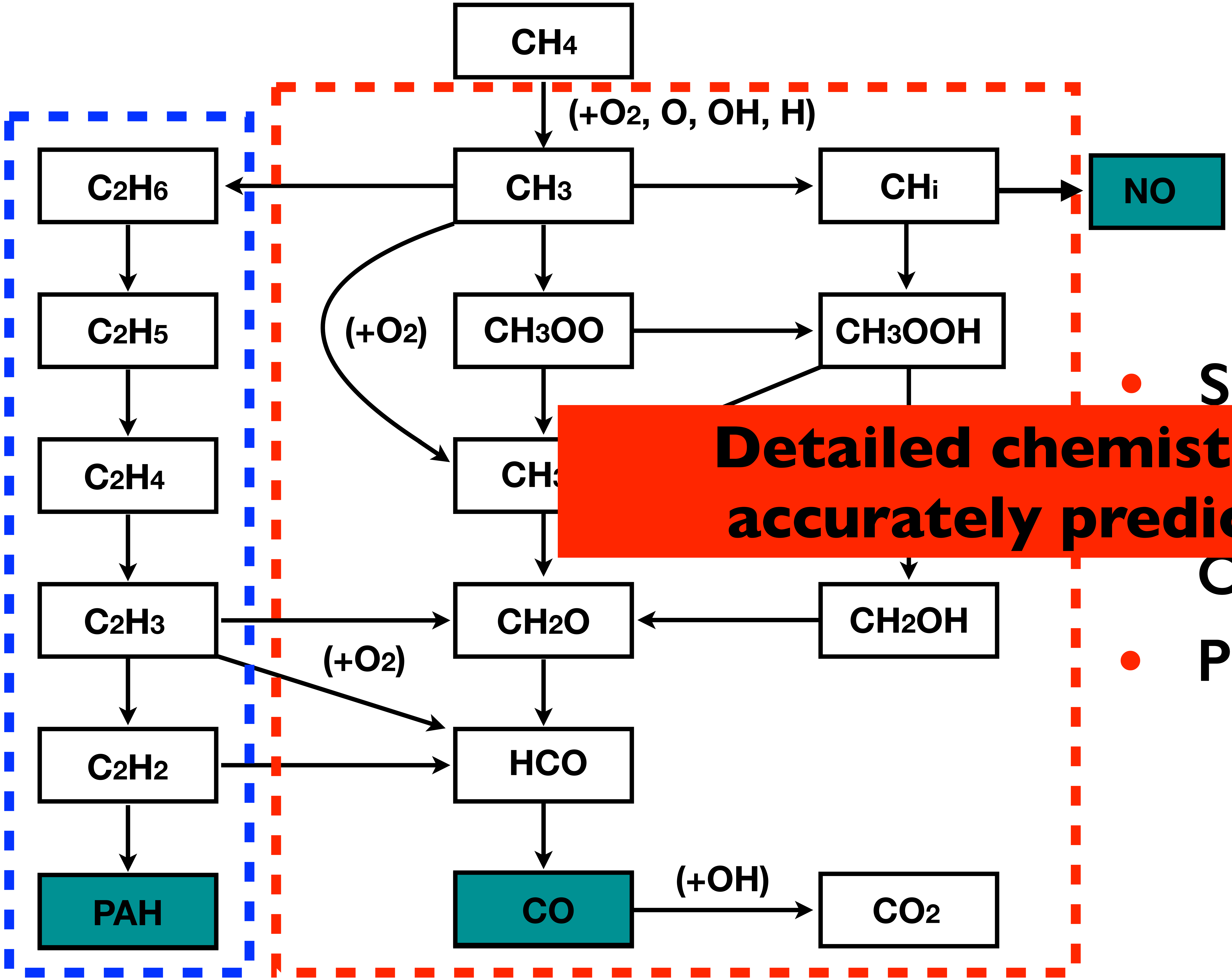

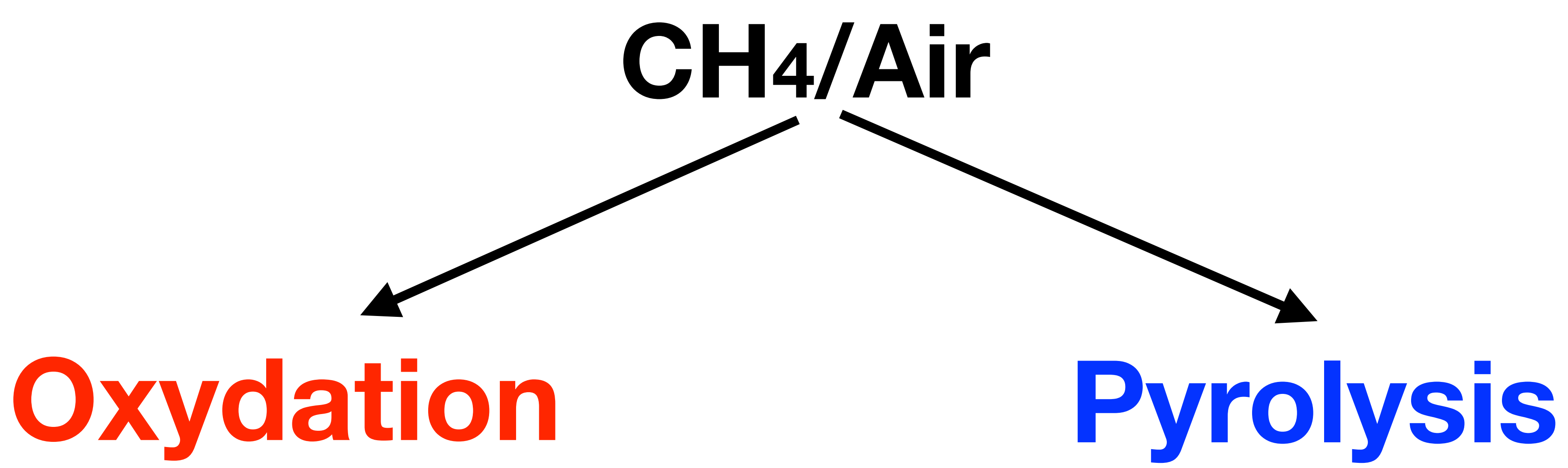

- Several path from $CH_4 \longrightarrow CO_2$

re
Oxydation

Detailed chemistry needed to accurately predict pollutants

- Pollutant formation :
  - CO
  - NO
  - PAH

E. Ranzi et al. (1994)
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Pollutant formation prediction in large scale application

➡ Turbulent flow field

➡ Air/Fuel stratification

➡ Multiple combustion regimes

➡ Heat losses etc…

CO :

➡ Intermediate / Product species

NO :

➡ Fast / Long time scales

➡ Slow recombination / Reburning

- Detailed chemistry too expensive

- Reduced order chemistry models needed to limit the simulation CPU cost

Chemistry modeling in LES

- Strategies employed in Large Eddy Simulation to reduce CPU cost associated to combustion chemistry modeling:

➡ ***Global optimized mechanisms***

Westbrook et al., (1981)
Jones et al., (1988)
Franzelli et al., (2010)

- Low CPU cost
- Temperature, flame speed

- Limited range of operating conditions
- Pollutant…

➡ ***Tabulated chemistry***

Peters (1984)
Gicquel et al., (2000)
Van Oijien et al., (2001)
Pierce and Moin (2005)
Fiorina et al. (2010)

- Detailed chemistry

- Flamelet regime
- Multiple coordinates, Flame index

➡ ***Systematically reduced chemistry:***

1. ***Skeletal***
2. ***Analytically reduced***

Luche (2003)
Lu and Law (2005)
P. Pepiot and H. Pitsch(2008)
Jaravel et al., (2016)

- Accurate flame structure description including pollutants

- High CPU cost
- Size scales with fuel complexity

Reduced order chemistry models in LES

- Define a new reduced transported species method:

Alternative method

Virtual chemistry (M. Cailler et al. 2017)

➡ **Build-up reduced chemical mechanisms from scratch**

➡ **Use virtual species and virtual reactions**

➡ **Build-up dedicated sub-mechanisms to predict flame quantities of interest.**

Virtual kinetic mechanisms

- **Virtual kinetic scheme composed by:**
  - N_s **virtual species** $\mathcal{V}_k$
  - N_r **virtual reactions**

$$\sum_{k=1}^{k=N_s} \alpha'_{ki}\mathcal{V}_k \rightarrow \sum_{k=1}^{k=N_s} \alpha''_{ki}\mathcal{V}_k \quad (i = 1, ..., N_r)$$

- The strategy relies on optimizing:
  - the **number of virtual species and virtual reactions**
  - **thermodynamic properties** of virtual species
  - **reaction rate parameters** of the virtual scheme

➡ **Species properties**

$$c_{pk}, h_k, \lambda_k, D_k$$

➡ **Kinetic rate parameters**

$$A_i, E_{ai}, F_i^k$$

optimization loop

Reference database computed with detailed chemistry:

- **0D Reactors**
- **Equilibrium calculations**
- **1D laminar calculations (premixed and/or non premixed, non-adibatic, etc…)**

M. Cailler, N. Darabiha, D. Veynante and B. Fiorina. Building-up virtual optimized mechanism for flame modeling. Proceeding of the Combustion Institute (2017)

Virtual optimized mechanisms methodology

$$\begin{cases} min(f(\underline{x}^v) - f(\underline{x}^d)) \\ \underline{x}^v_- < \underline{x}^v < \underline{x}^v_+ \end{cases}$$

$f(\underline{x})$ Selected flame quantities

$\underline{x}$:
- Thermodynamic
- Transport
- Kinetic

Detailed chemistry mechanism

Computation of representative configurations

Reference flame library :

★Equilibrium computations

★1D-flame archetypes:

- 1-D unstretched premixed flames
- 1-D counterflow diffusion flames
- 1-D non-adiabatic flames (Burner-Stabilized)
- etc…

Optimization loop

Navier Stokes equations solver

Main mechanism for flame/ flow field interaction prediction

★ Mixture properties
★ Temperature
★ Density
★ Heat Release

Sub-mechanisms for pollutant species

CO block

NO_x block

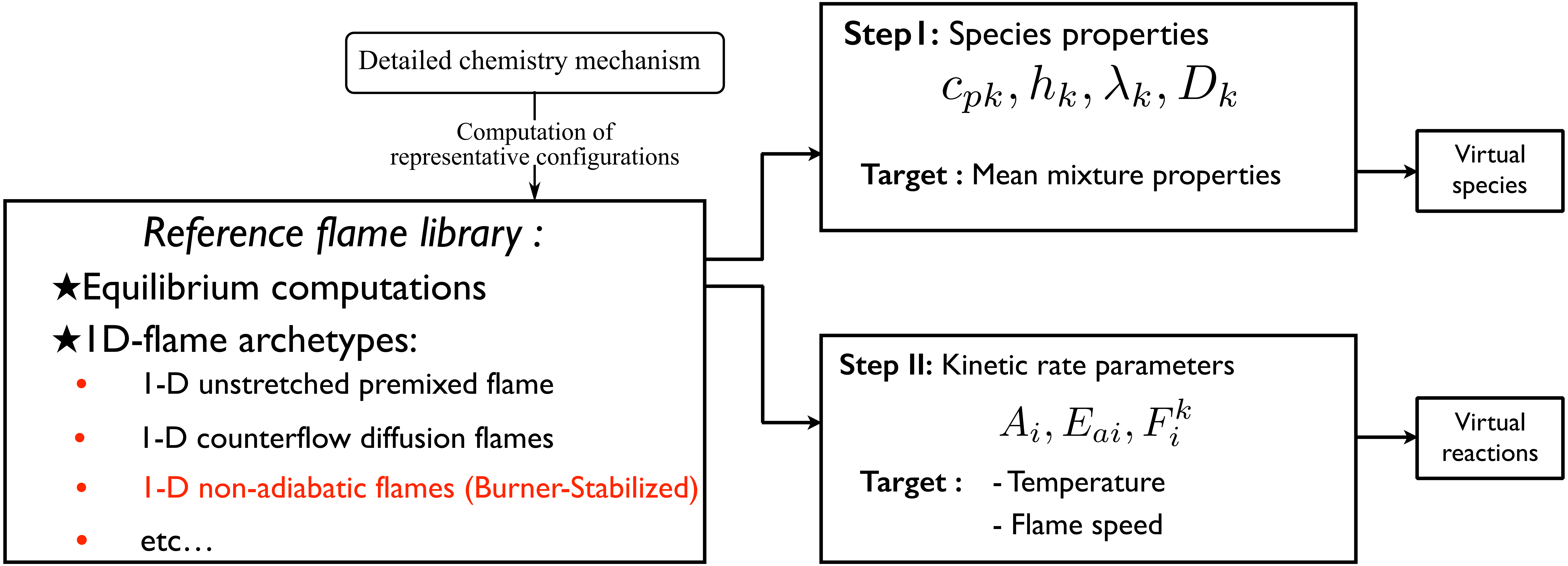
PAH block

Virtual optimized mechanisms

Main virtual mechanism generation procedure

$$\alpha_F F + \alpha_{Ox} Ox + \alpha_D D \rightarrow \alpha_I I + \alpha_D D \quad (1)$$

$$I \rightarrow \sum_{k=1}^{N_P^v} \alpha_{P_k} P_k \quad (2)$$



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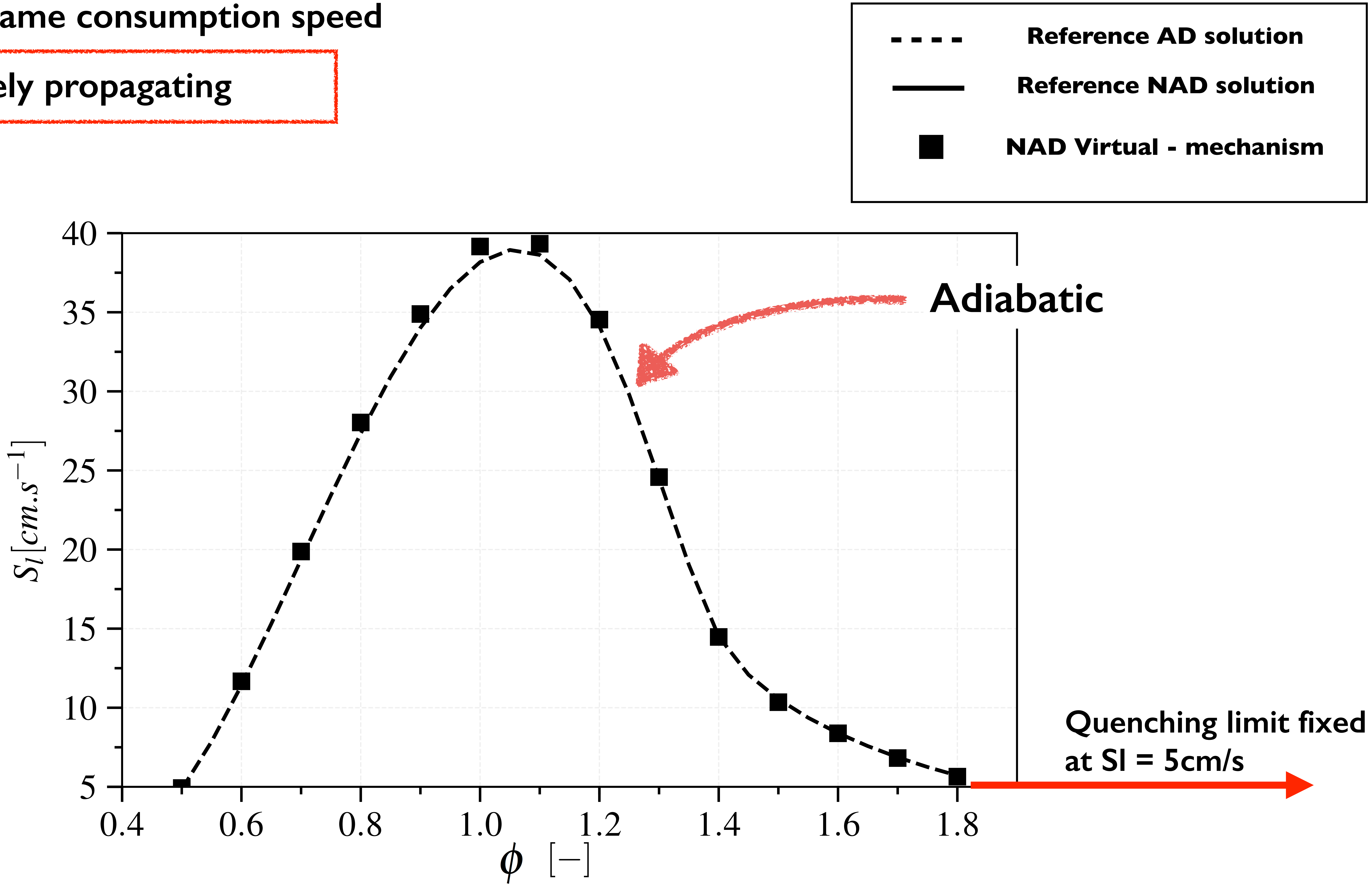
Virtual optimized chemistry: Adiabtic/Non-adiabatic conditions

Validation versus the reference solution (GRI3.0)

- Laminar flame consumption speed
  - Freely propagating



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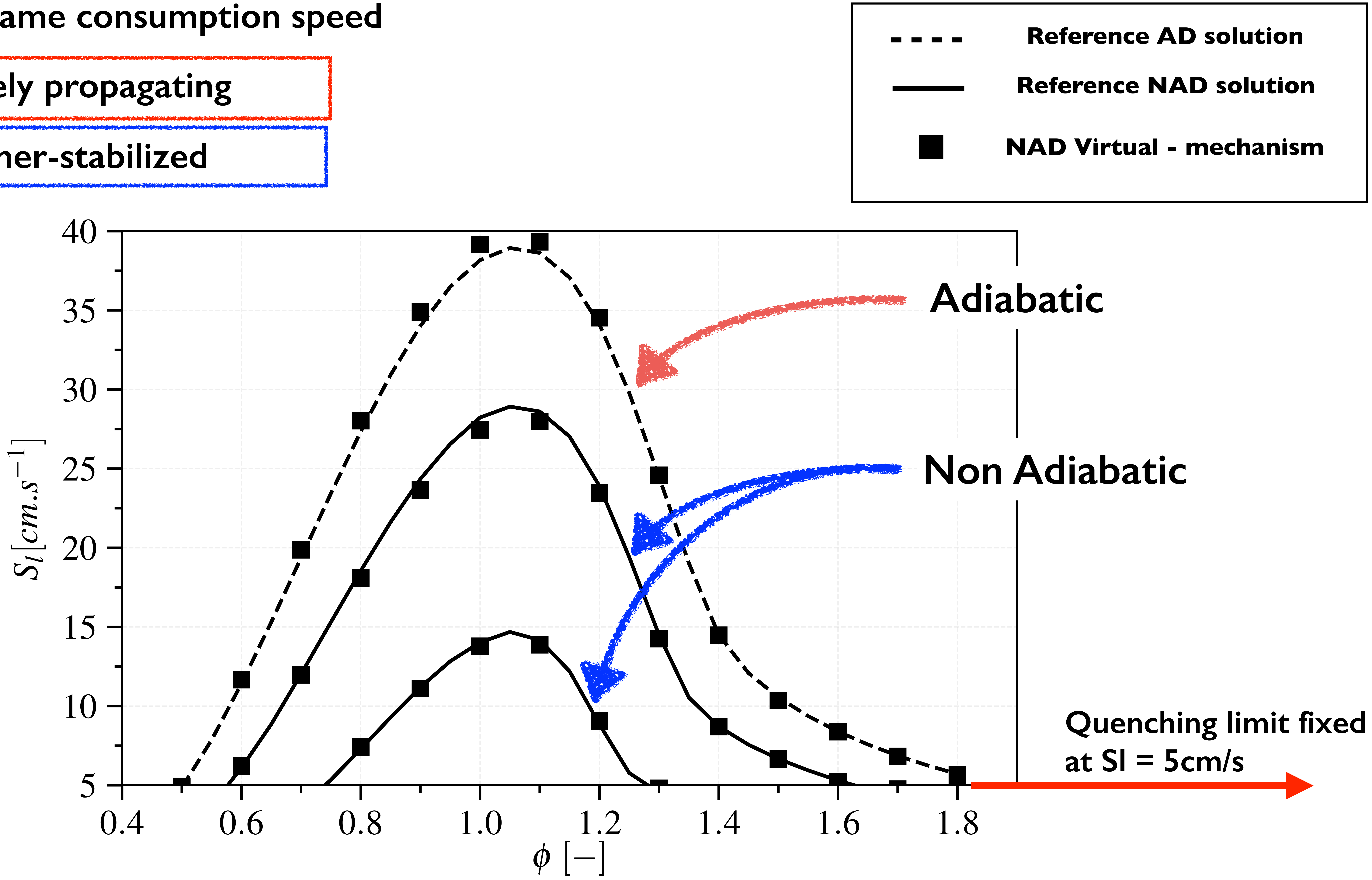
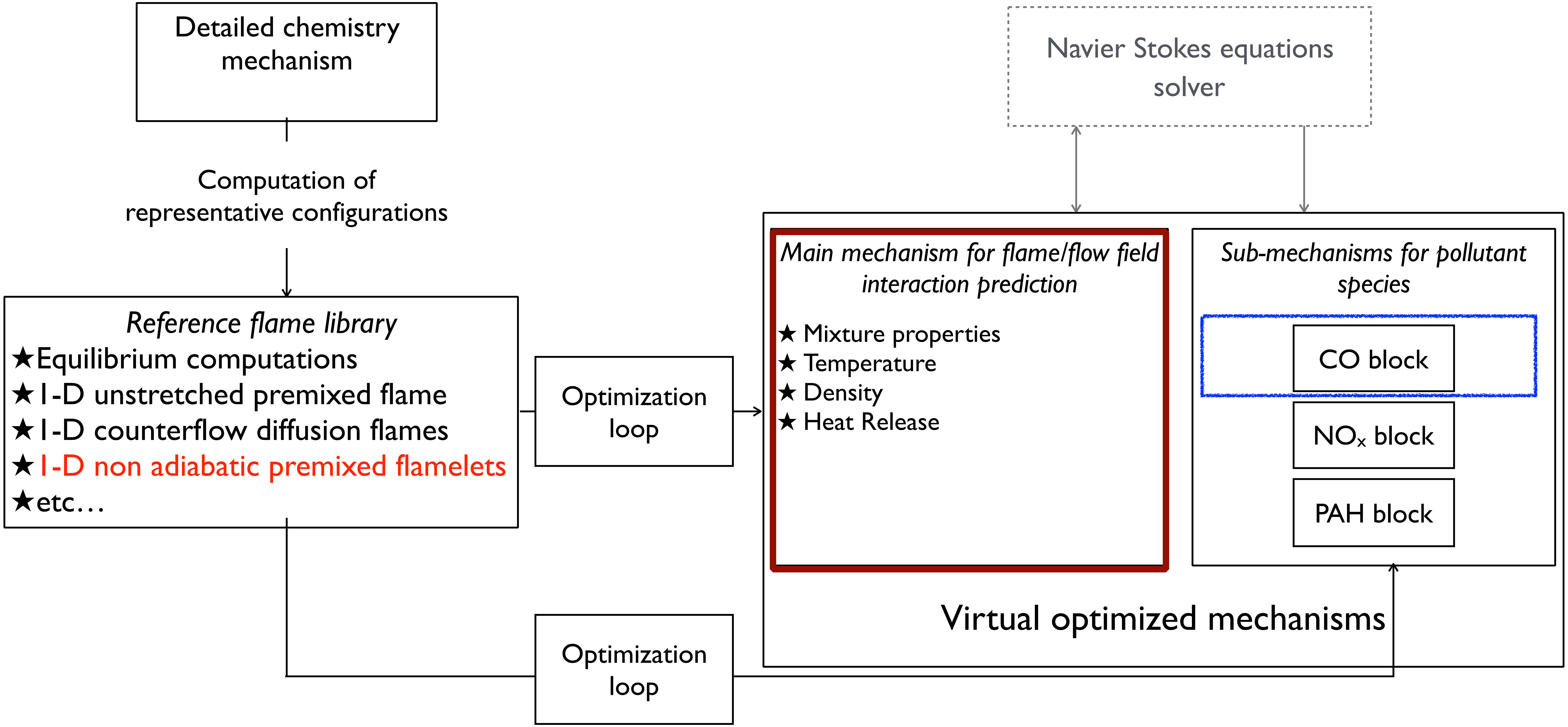


Virtual optimized mechanisms: pollutants (CO)



CO pollutant sub-mechanism

- **3 step mechanism :**

$$\alpha_F F + \alpha_{Ox} Ox \rightarrow \alpha CO + (1-\alpha) \boxed{V_1} \quad (3)$$

$$F + \boxed{V_1} \rightarrow F + CO \quad (4)$$

$$CO \leftrightarrow \boxed{V_2} \quad (5)$$

- **Rate of progress**

$$q_3 = A_3 f_3(\phi, \Delta h) exp\left(\frac{-E_{a,3}}{RT}\right) [F]^{F_F^3} [Ox]^{F_{Ox}^3}$$

$$q_4 = A_4 f_4(\phi, \Delta h) exp\left(\frac{-E_{a,4}}{RT}\right) [F]^{F_F^4} [V_1]^{F_{V_1}^4}$$

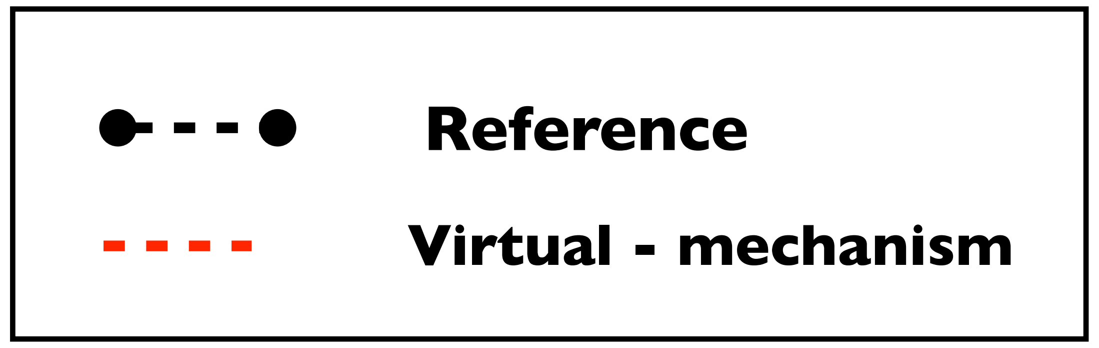
$$q_5 = A_5 f_5(\phi, \Delta h) exp\left(\frac{-E_{a,5}}{RT}\right) \left([CO]^{F_{CO}^5} [V_2]^{F_{V_2}^5} - \frac{[CO]^{R_{CO}^5} [V_2]^{R_{V_2}^5}}{K_{c,5}^v(\phi, \Delta h)}\right)$$

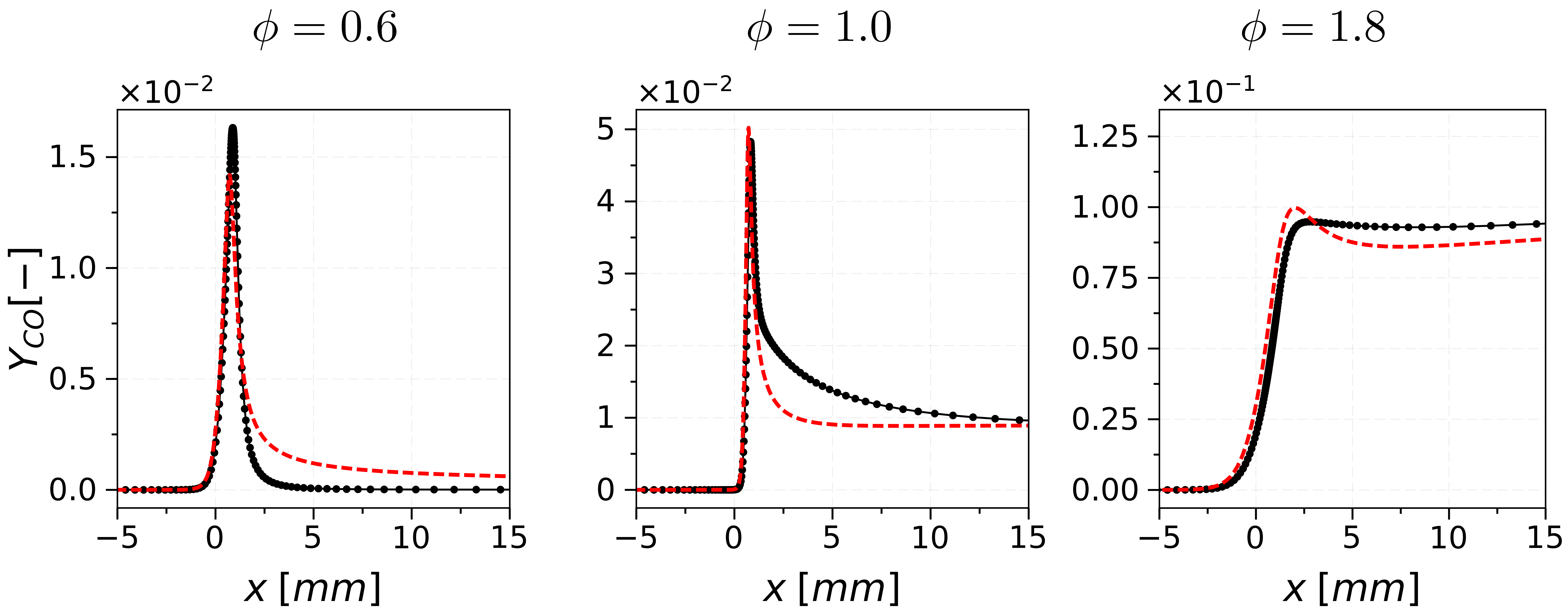
capture Yco at equilibrium

Validation in adiabatic conditions

CH4/air combustion at atmospheric pressure and T fresh of 300K

1D Premixed laminar flames





- M. Cailler, N. Darabiha, D. Veynante and B. Fiorina. Building-up virtual optimized mechanism for flame modeling. Proceeding of the Combustion Institute (2017)
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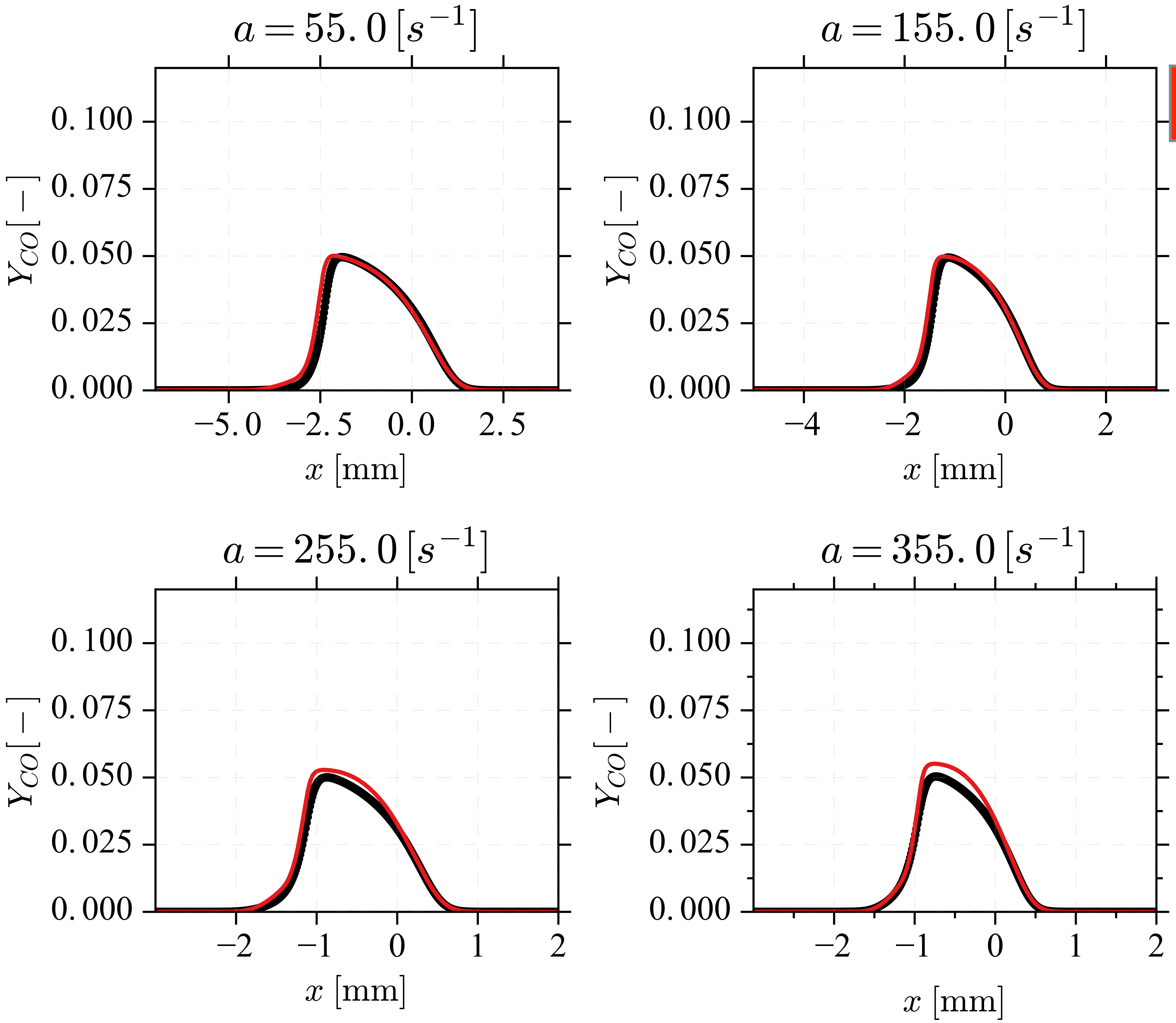

1D Non-Premixed flames

Reference

Virtual - mechanism

➡ No flame index

➡ No multiple chemical table coordinates

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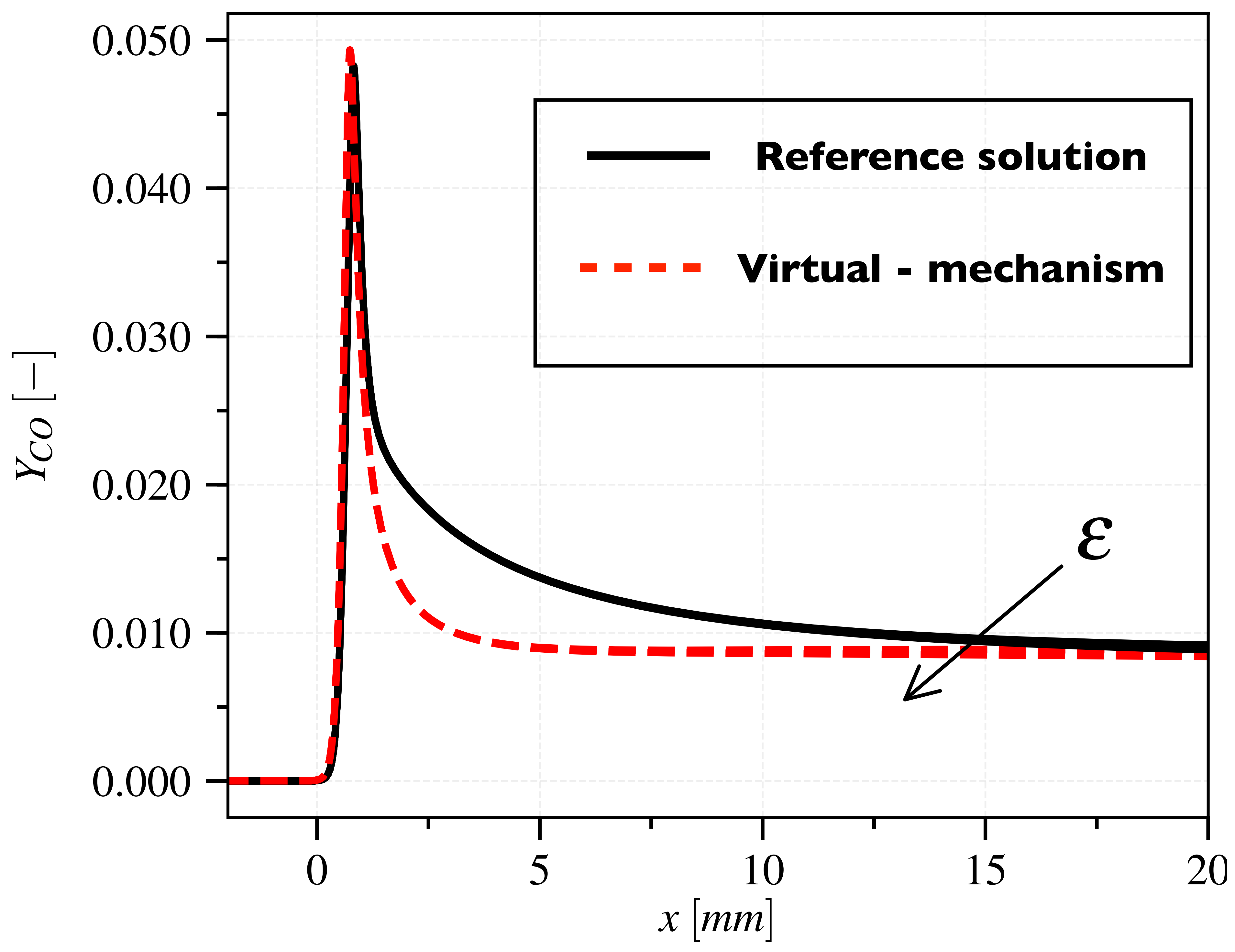
1-D premixed flame submitted to radiative heat losses

- A radiation sink is added to the energy balance equation of the 1-D flame solver

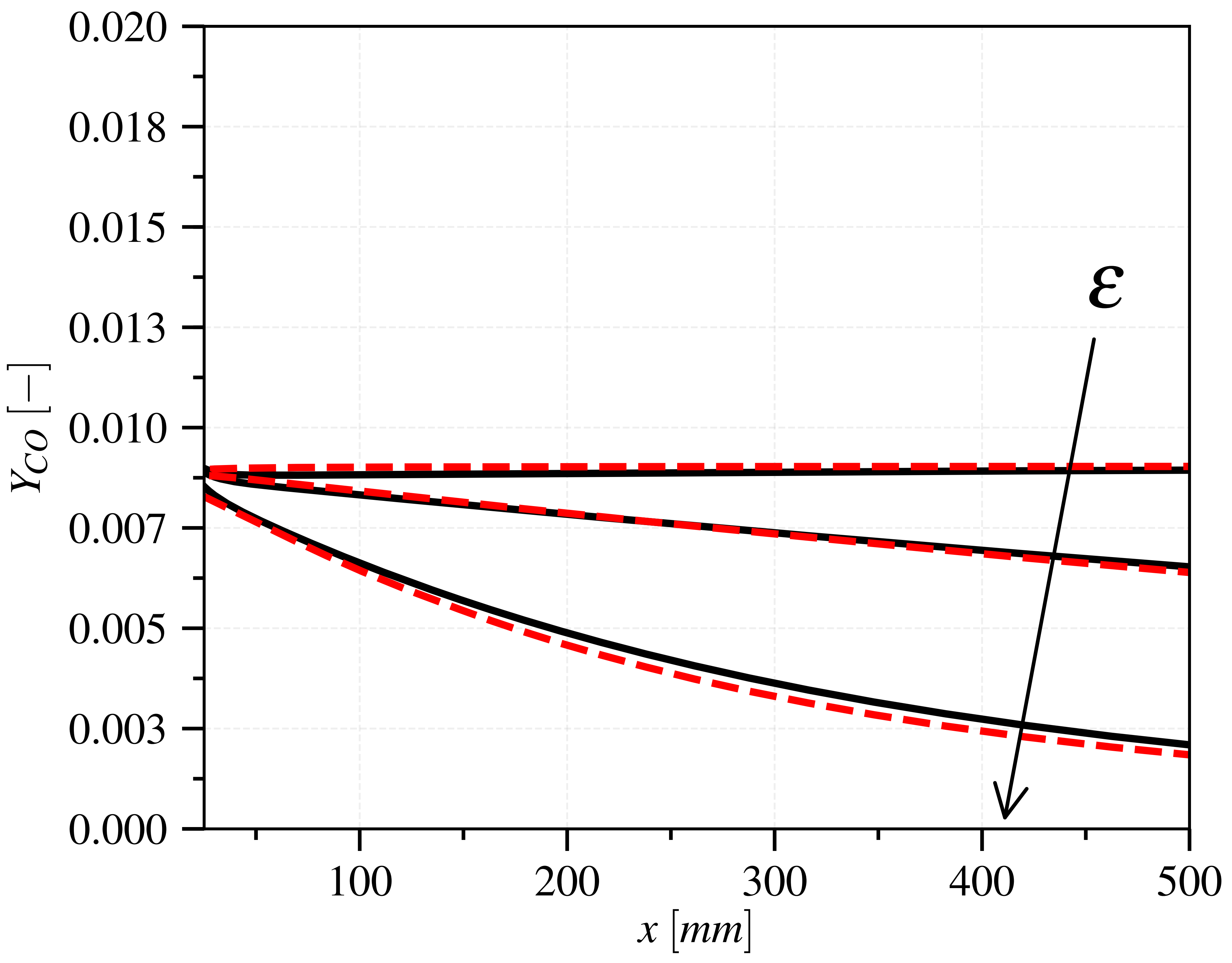
$$u\rho c_p \frac{dT}{dx} - \frac{d}{dx}\left(\lambda \frac{dT}{dx}\right) + \sum_k \left(\rho Y_k V_k c_{p_k}\right)\frac{dT}{dx} + \sum_k h_k \dot{\omega}_k + \sigma\epsilon\left(T^4 - T_0^4\right) = 0$$

1D Non-adiabatic

➡ CO mass fraction / Flame Front



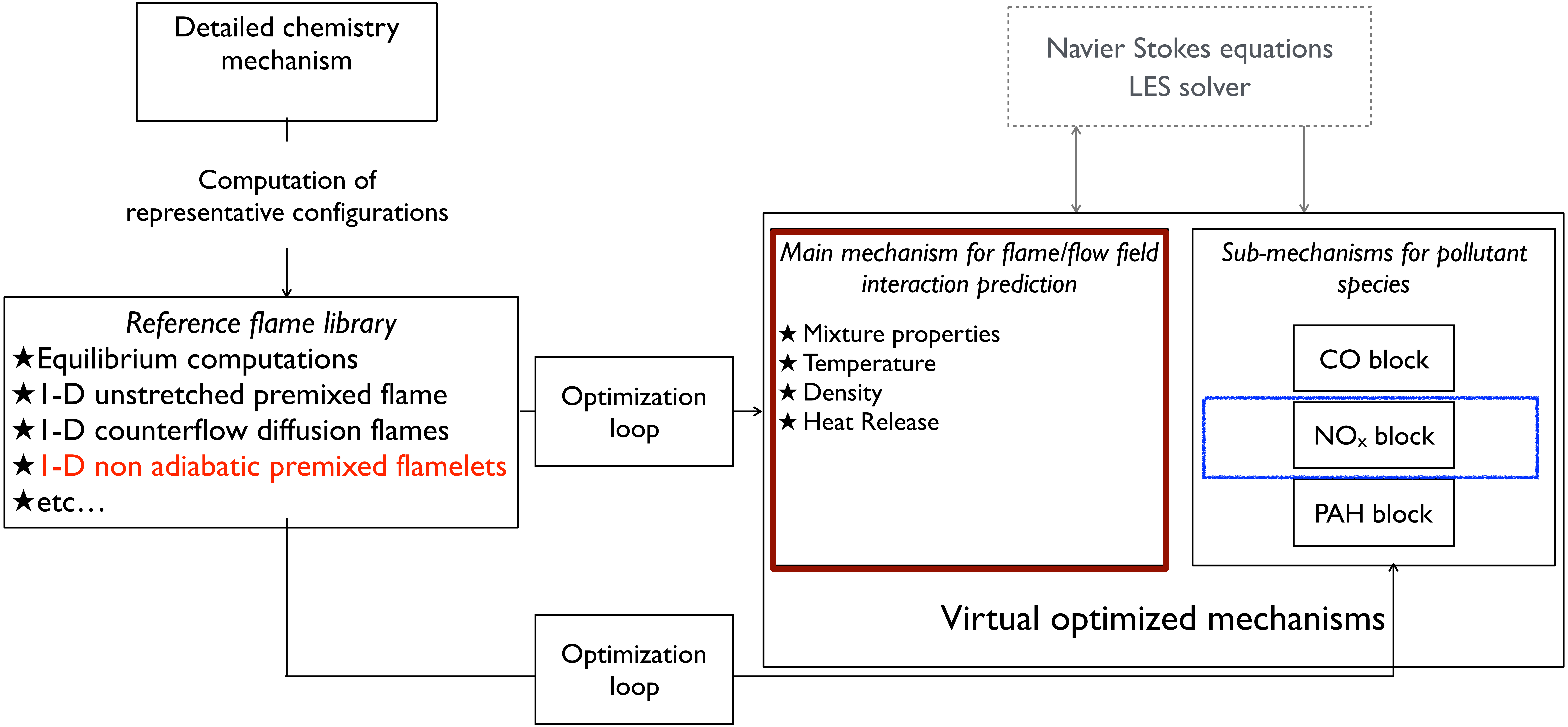
➡ CO mass fraction / Post Flame



➡ No enthalpy coordinate

- CO production well captured in the post-flame region / local equilibrium change

Virtual optimized mechanisms: pollutants (NO)



Virtual sub-mechanism for NO prediction

NO sub-mechanism :

- **Challenge : multiple time scale to capture + post-flame reburning effects**

$$\alpha_F F + \alpha_{Ox} Ox \rightarrow \alpha V_1 + (1-\alpha-\gamma) V_2 + \gamma V_3 \quad (3)$$

$$V_1 + F + Ox \rightarrow \beta NO + (1-\beta) V_2 + F + Ox \quad (4)$$

$$F + NO \rightarrow F + V_2 \quad (5)$$

→ **Flame Front / Fast NO formation**

$$V_2 \leftrightarrow NO \quad (6)$$

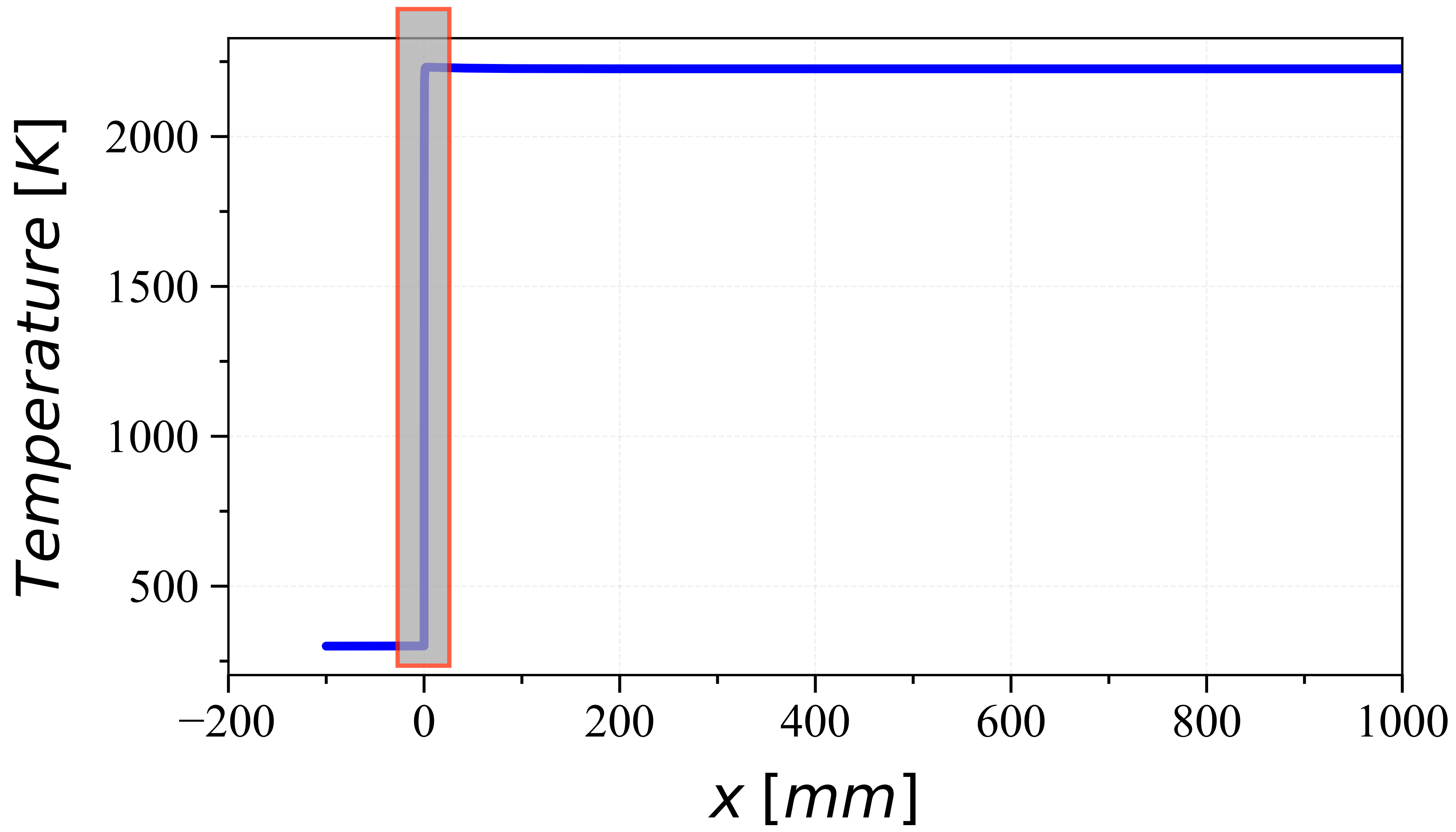
$$V_3 \rightarrow NO \quad (7)$$

$$V_3 \rightarrow V_2 \quad (8)$$

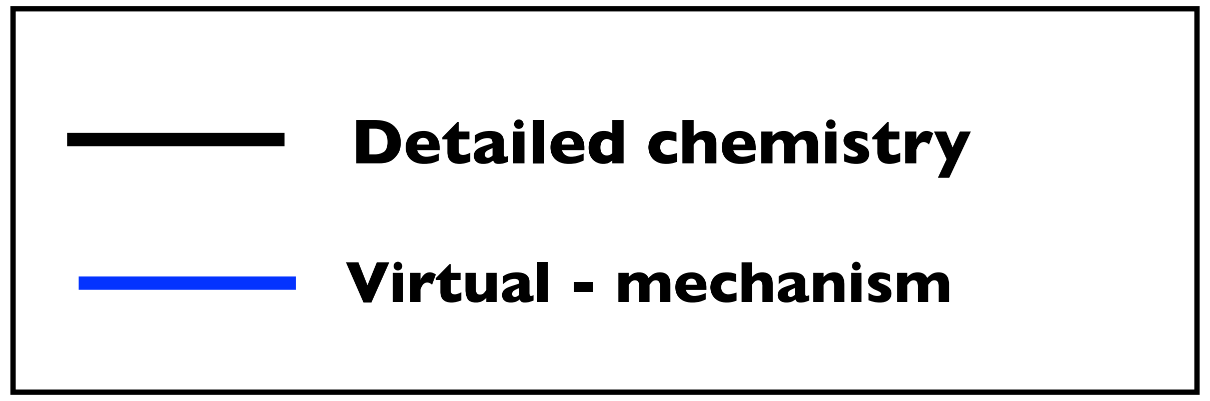
→ **Post Flame / Slow NO formation and consumption**

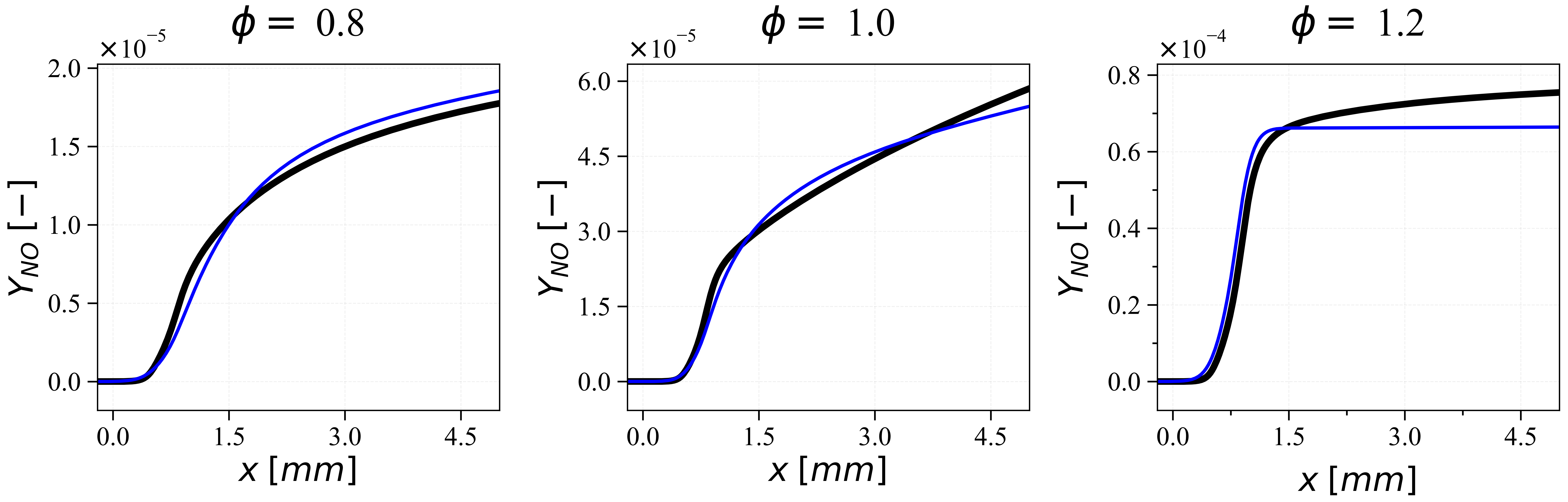
Virtual sub-mechanism for NO prediction

Validation of the results :



Flame Front / Fast NO formation

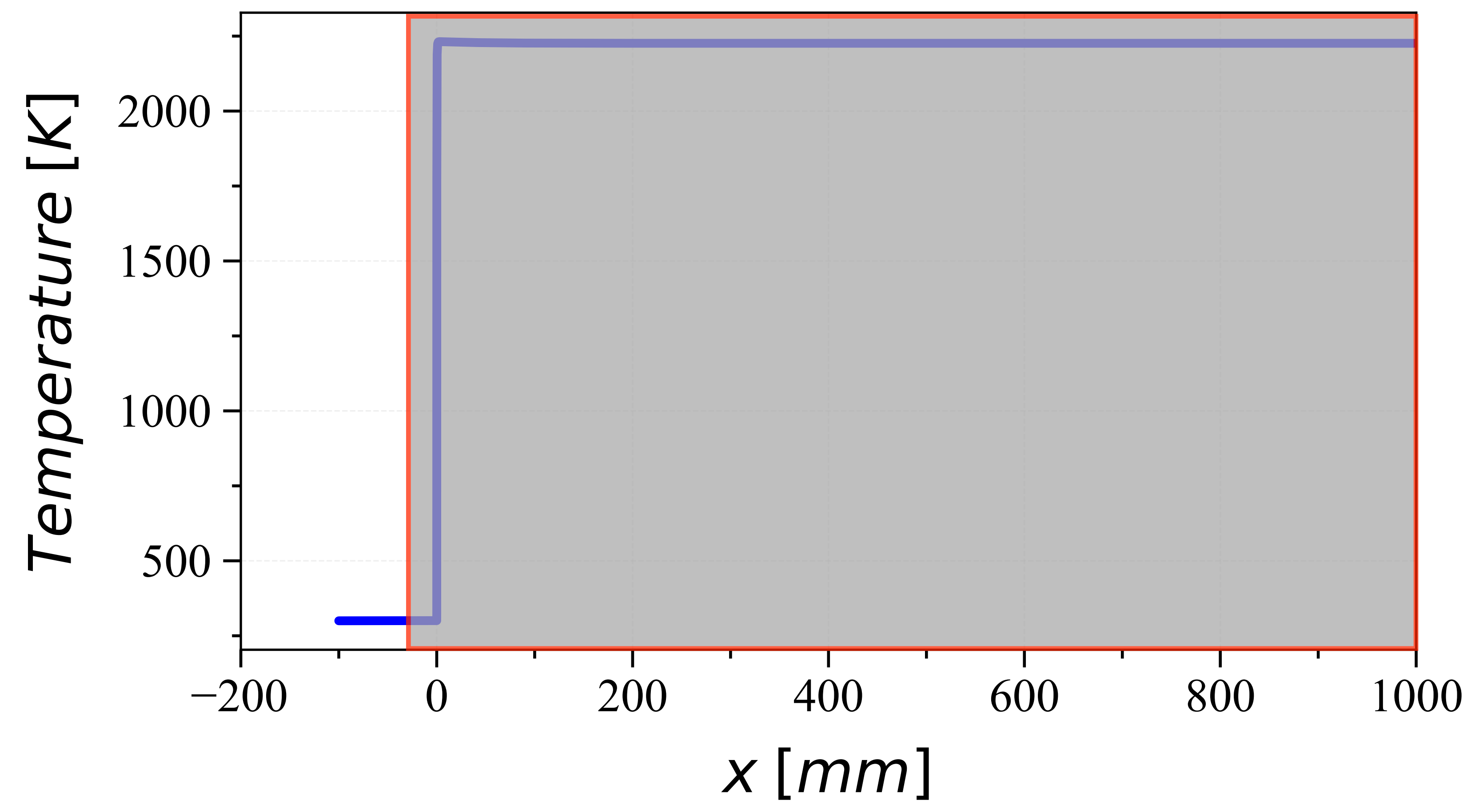


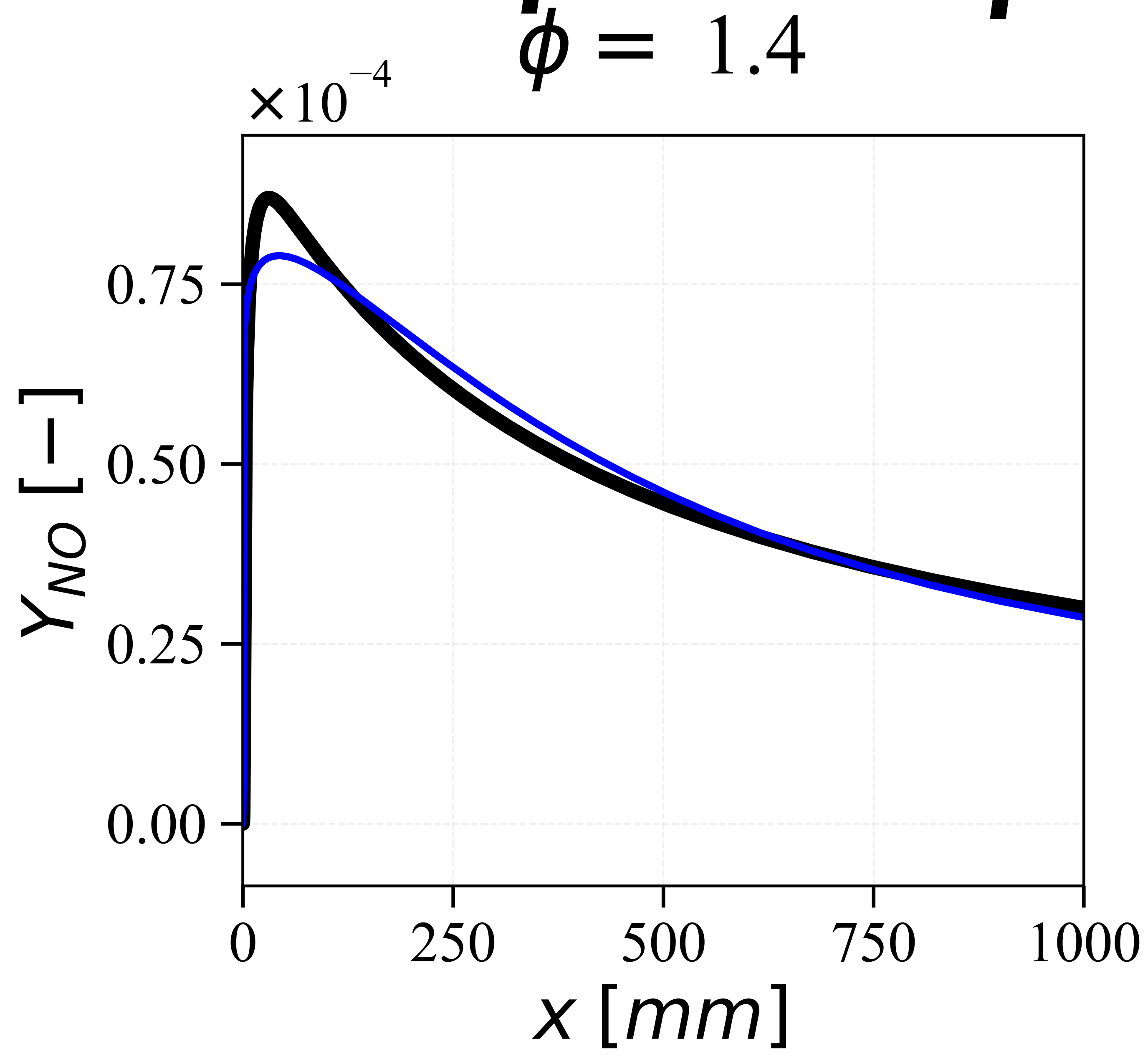


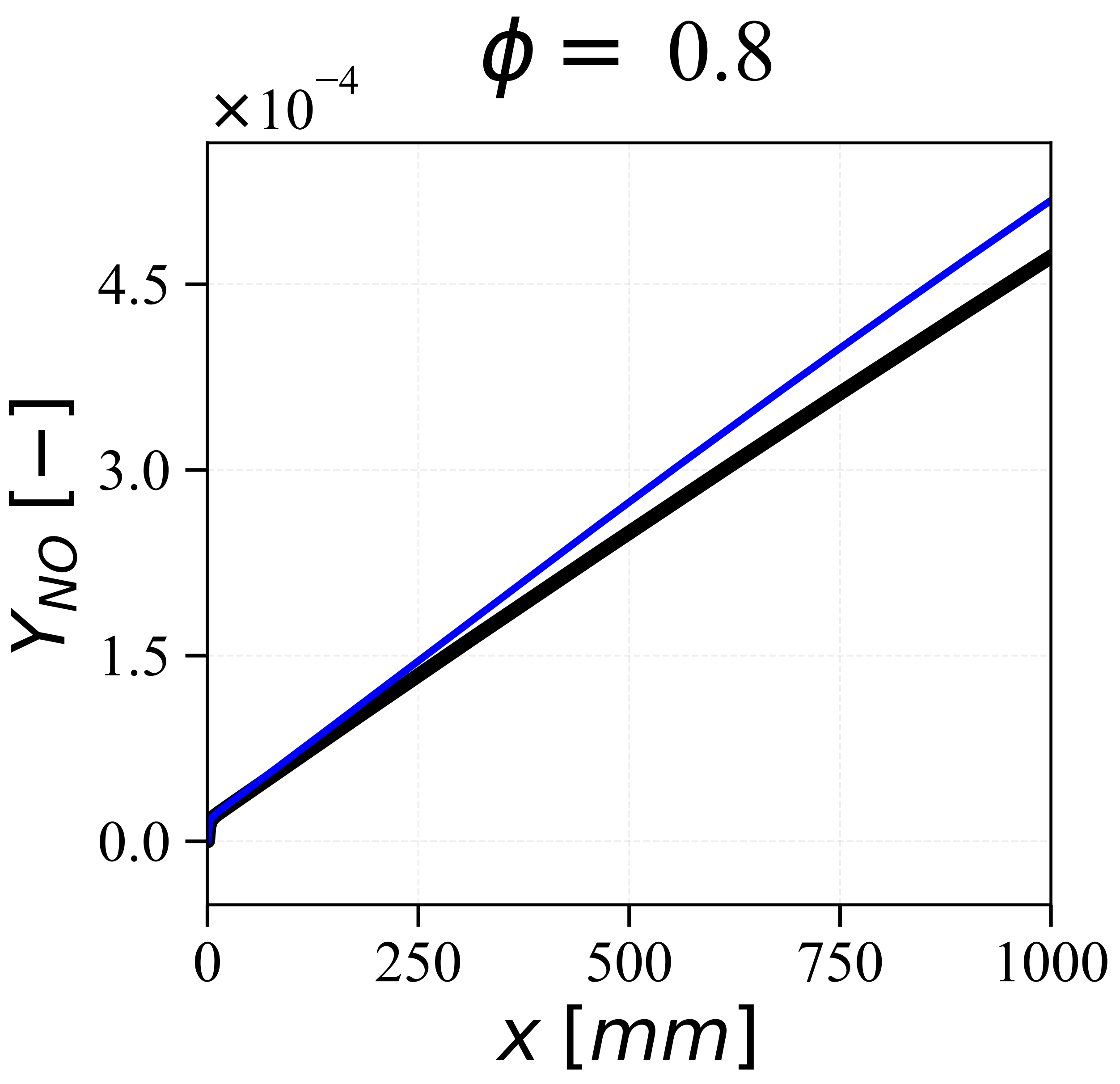
Virtual sub-mechanism for NO prediction

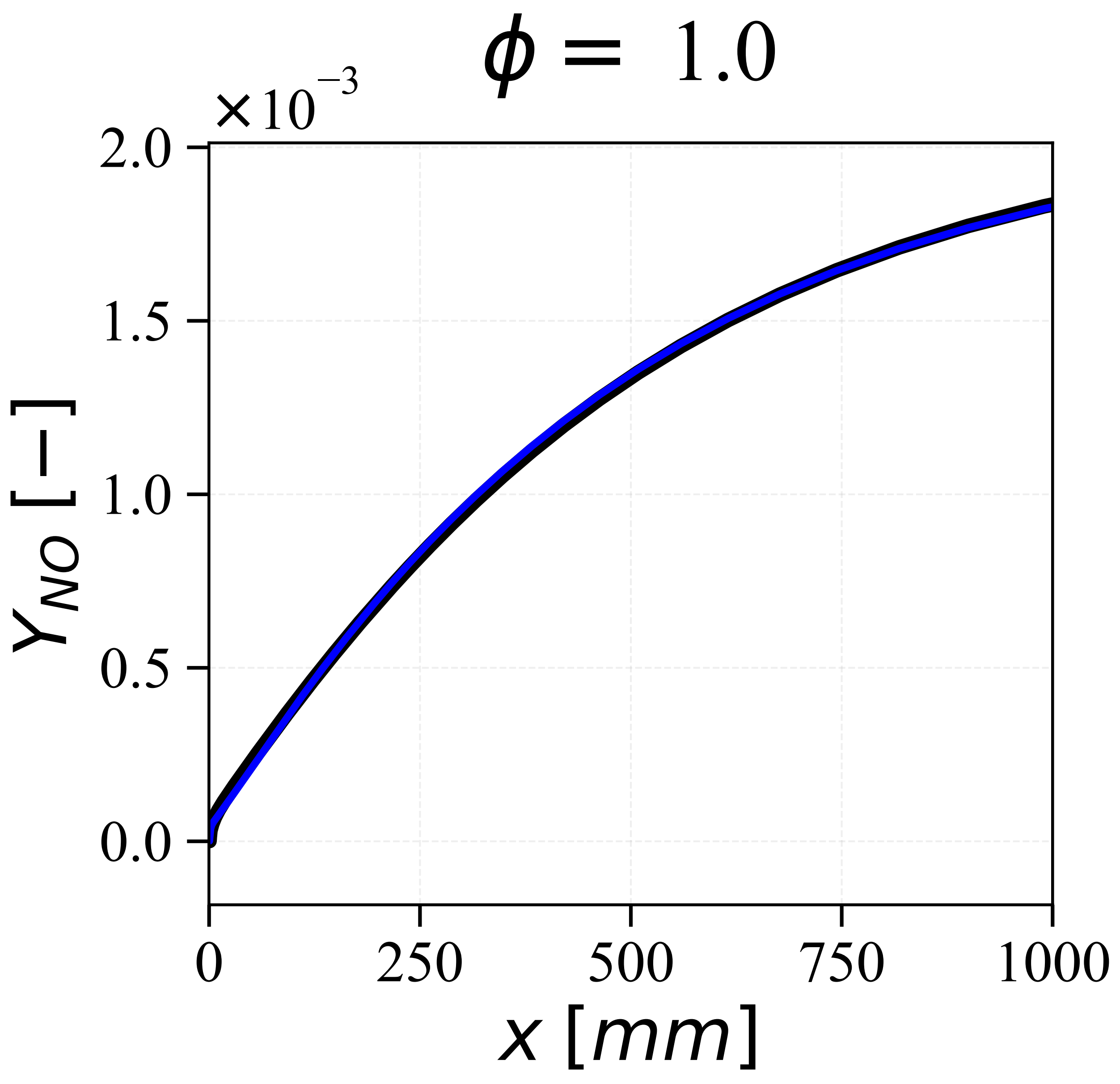
Validation of the results :

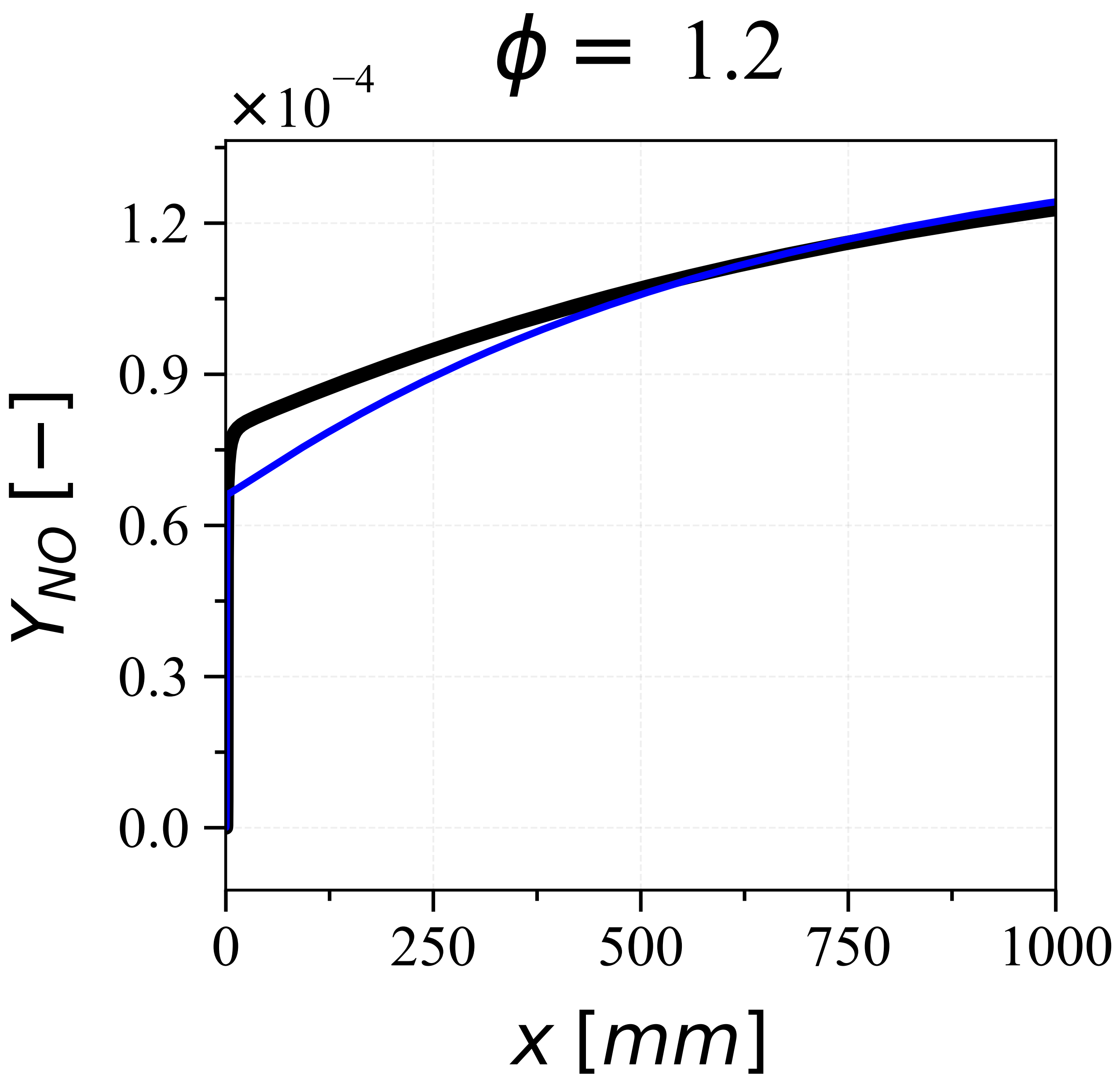
Post Flame / Slow NO formation







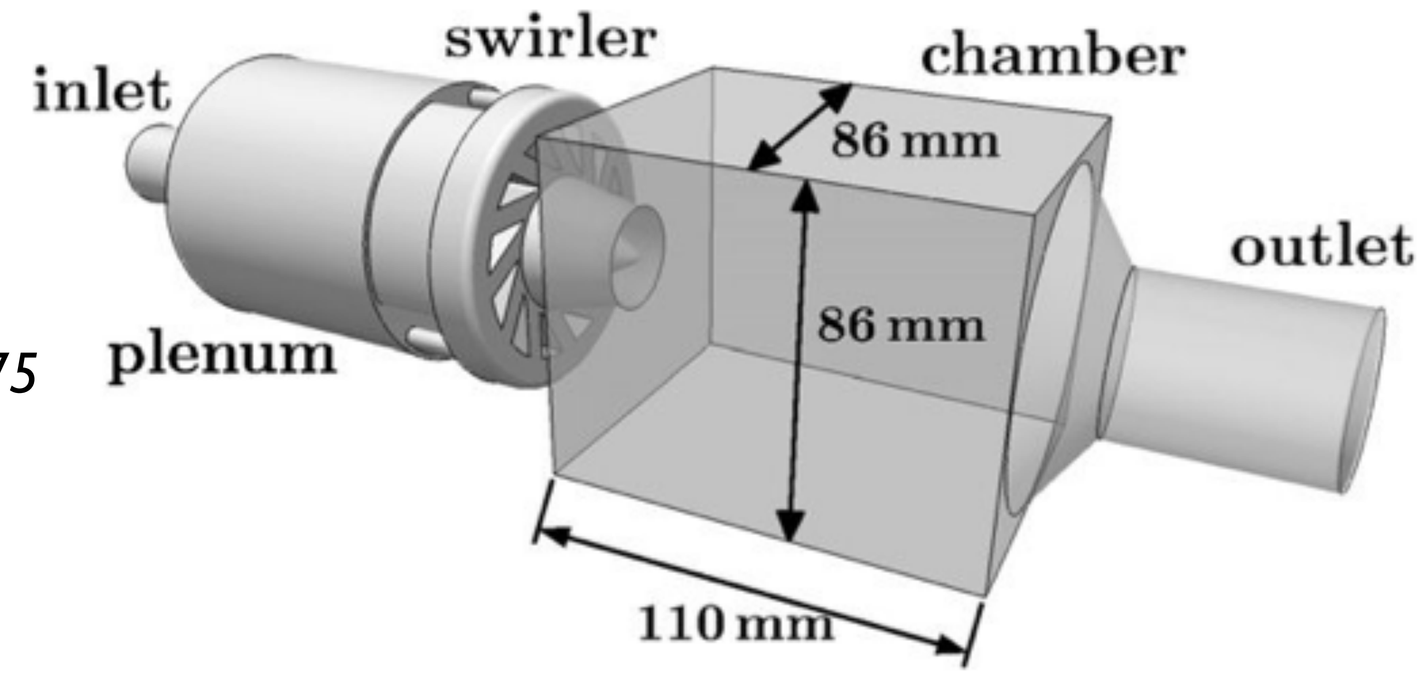




LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

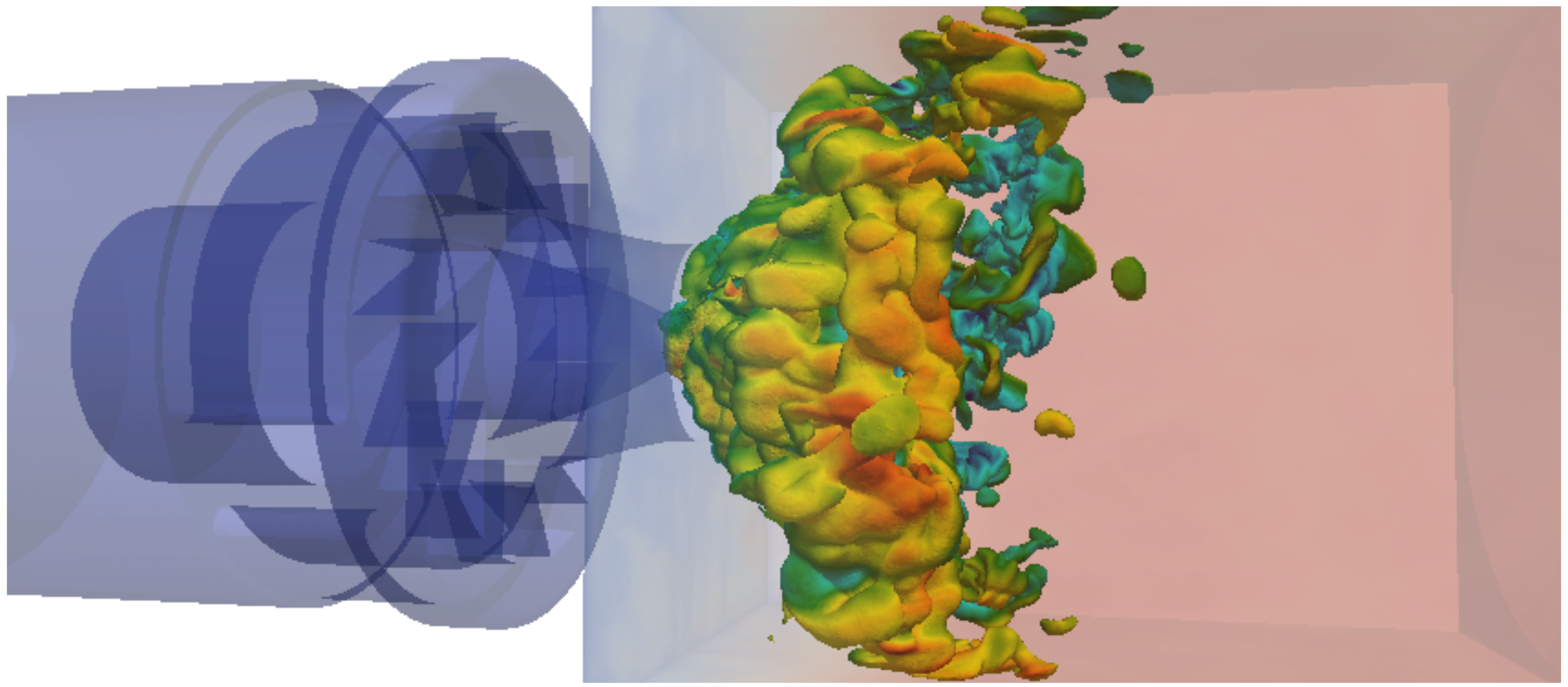
- **Test non adiabatic virtual chemistry in a 3-D LES turbulent calculation**
  - Turbulent premixed swirled burner (Meier et al., Combust. Flame, 2007)
- Previous numerical works reproduce fairly well flow dynamics as well as the mean flame front position

B. Franzelli, E. Riber, L.Y. Gicquel, T. Poinsot, Combust. Flame 159 (2012) 621–637
S. Roux, G. Lartigue, T. Poinsot, U. Meier, C. Bérat, Combust. Flame 141 (2005) 40–54
V. Moureau, P. Domingo, L. Vervisch, Combust. Flame 158 (2011) 1340–1357
B. Fiorina, R. Vicquelin, P. Auzillon, N. Darabiha, O. Gicquel, D. Veynante, Combust. Flame 157 (2010) 465–475
R. Mercier, V. Moureau, D. Veynante, B. Fiorina, Proc. Combust. Inst. 35 (2015) 1359–1366
P. S. Volpiani, T. Schmitt, D. Veynante, Combust. Flame 180 (2017) 124–135



Geometry of the Preccinsta burner
(Moureau et al., Combust. Flame, 2011)

Wall heat losses



- But problems for Temperature and CO prediction in the ORZ, attributed to chamber wall heat losses

LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

Numerical set-up:

- Wall temperature profile not experimentally provided
- Wall Dirichlet boundary conditions provided by CORIA group (*P.Benard et al. , 2018*) by numerical simulation conducted with a reference 17 species skeletal scheme (Sankaran et al. 2007)
- YALES2 (**CORIA** *V. Moureau et al. 2011*)
- Combustion chemistry modeled using non adiabatic virtual mechanisms **(**two-step main mechanism and the CO dedicated sub-mechanism **)**
- Turbulence/Flame interaction: Thickened Flame model for LES (*Colin et al., 2000*)

$$\frac{\partial \bar{\rho}\widetilde{Y_k}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\widetilde{u_i}\widetilde{Y_k}\right) = \frac{\partial}{\partial x_i}\left(\left[F\,\Xi_\Delta \frac{\mu}{Sc} + (1-S)\frac{\mu_t}{Sc_t}\right]\frac{\partial \widetilde{Y_k}}{\partial x_i}\right) + \frac{\Xi_\Delta}{F}\widetilde{\dot{\omega}_k}$$

- Sub-grid flame wrinkling (*Charlette et al., 2002*) with β=0.5.
- Flame sensor based on virtual species source term. (*Cailler et al. 2017*)

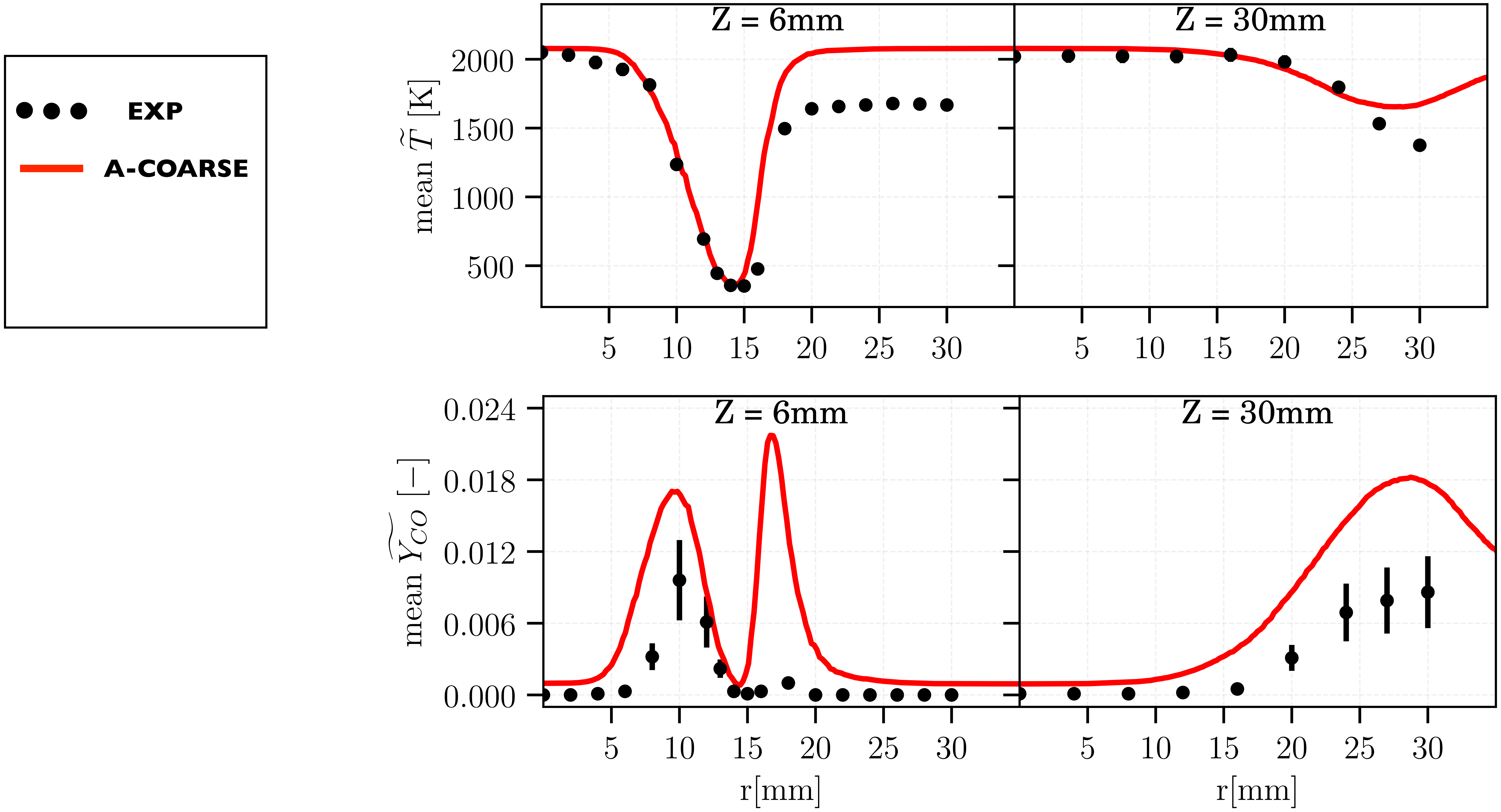
LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

➡ **Simulation results : Instantaneous Heat release rate**

Adiabatic Coarse 2.7M nodes

LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

Simulation results : Temperature / CO Reynolds statistics



LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

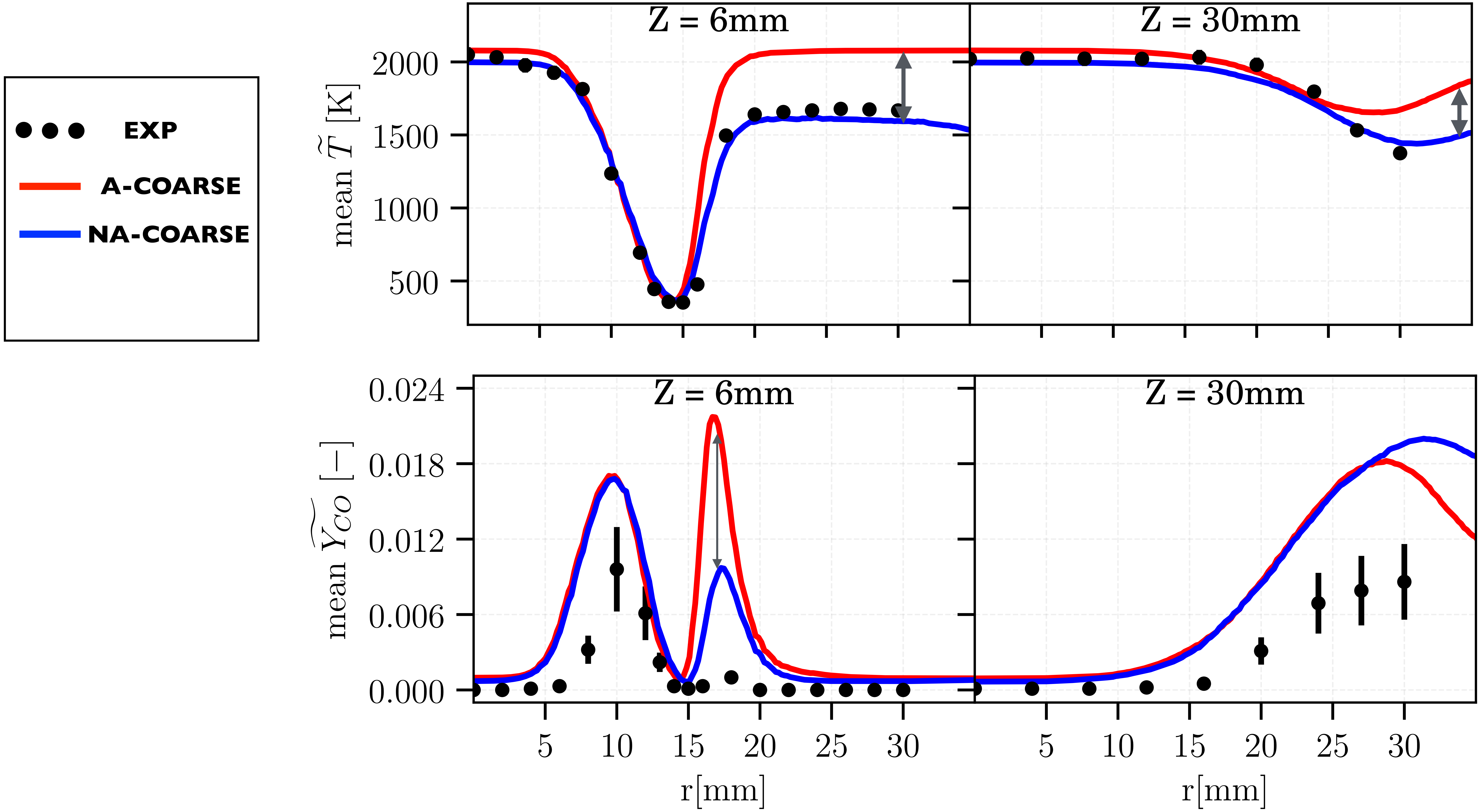
➡ **Simulation results : Instantaneous Heat release rate**

Adiabatic Coarse 2.7M nodes

N-Adiabatic Coarse 2.7M nodes

LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

Simulation results : Temperature / CO Reynolds statistics



LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

➡ **Simulation results : Instantaneous Heat release rate**

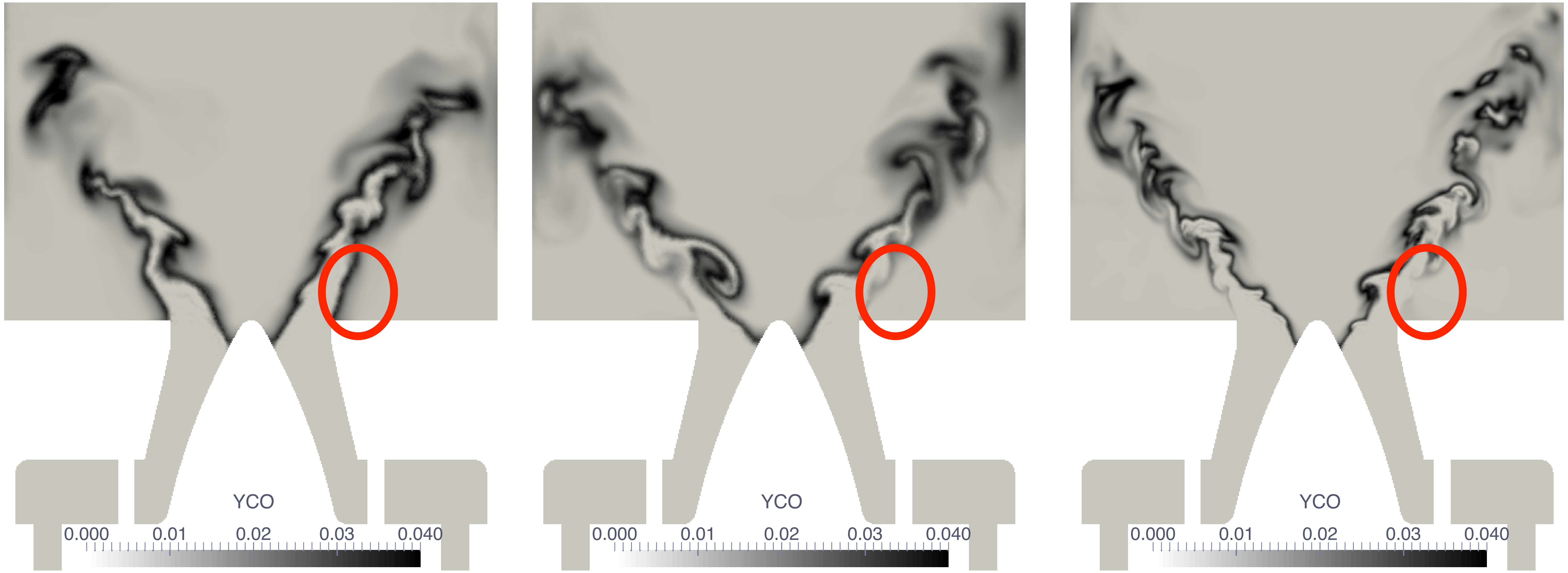
Adiabatic Coarse 2.7M nodes | N-Adiabatic Coarse 2.7M nodes | N-Adiabatic Fine 20.9M nodes

Transition from a M shape flame toward V shape flame due to heat losses and flame resolution improvement

LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

➡ Simulation results : Instantaneous CO filtered mass fraction

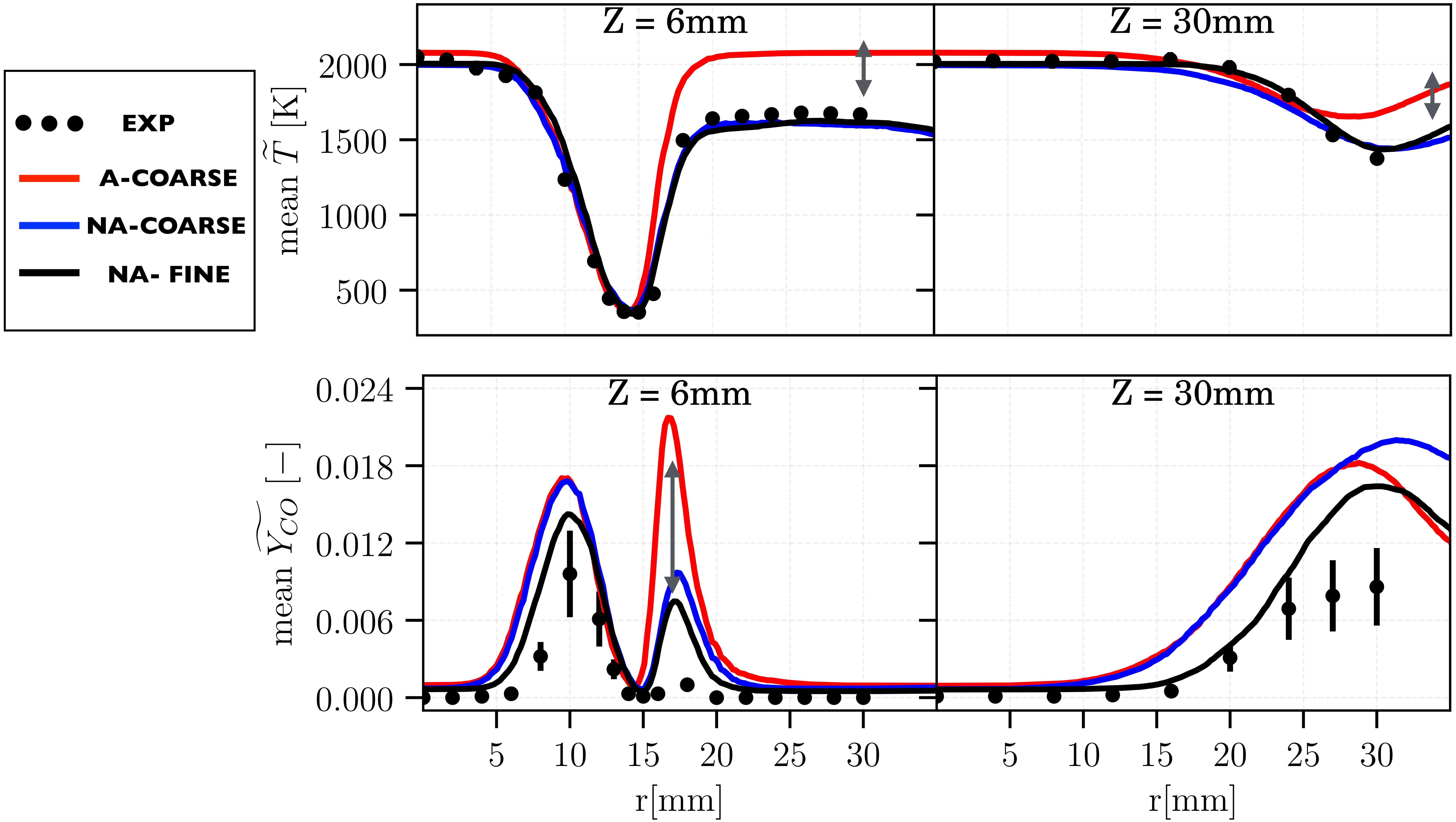
Adiabatic Coarse 2.7M nodes | N-Adiabatic Coarse 2.7M nodes | N-Adiabatic Fine 20.9M nodes



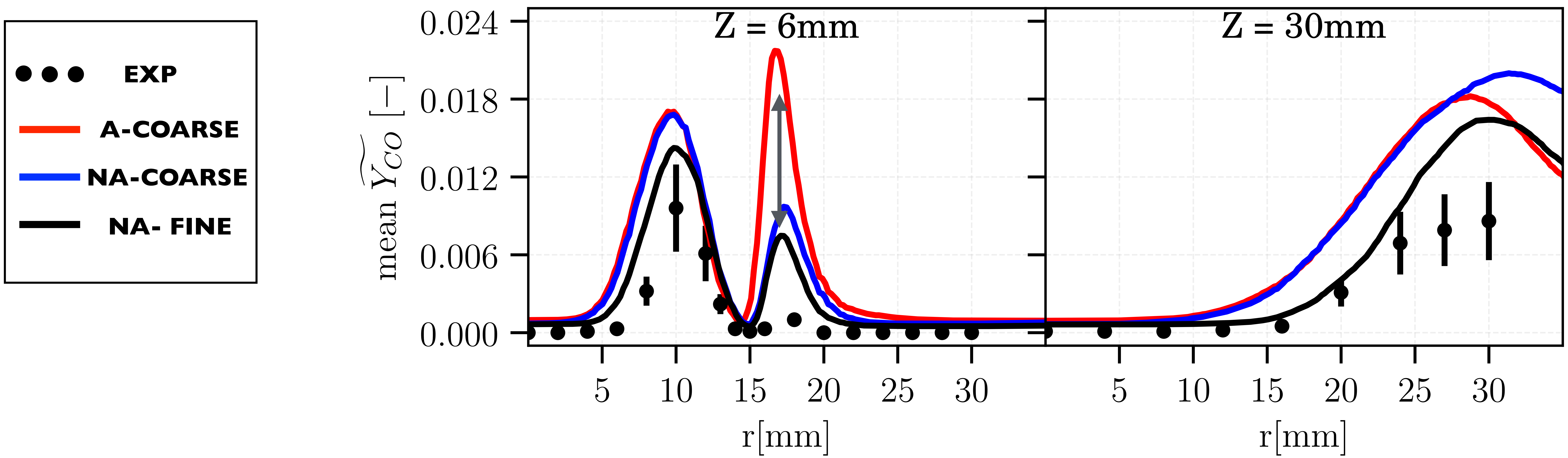
- CO formation impacted by heat losses on the external branch of the flame
- CO is sensitive to mesh resolution.

LES of a non-adiabatic turbulent premixed flame (Preccinsta burner)

Simulation results : Temperature / CO Reynolds statistics



CO-prediction impacted by the turbulent combustion model (Preccinsta burner)



- **Combined effect of Thickening factor and Efficiency function on intermediate filtered species prediction (for example CO)**

Benard, P., Lartigue, G., Moureau, V., and Mercier R., Large-Eddy Simulation of the lean-premixed PRECCINSTA burner with wall heat losses Proceedings of the Combustion Institute, 2018.

R. Mercier, C. Mehl, B. Fiorina and V. Moureau. Filtered Wrinkled Flamelets model for Large-Eddy Simulation of turbulent premixed combustion, Submitted to Combustion and Flame(2018).

Conclusion

- Reduced combustion chemistry model that allows pollutants prediction (CO / NO)
- Virtual chemistry validated in the LES context including heat losses
- Mis-prediction of CO attributed to the turbulent combustion model
- The size of the virtual chemistry mechanisms does not change if the complexity of the system increases:
  - heat losses
  - multiple flame regimes
  - different fuels

Thank you for your attention

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