High-fidelity CFD simulation & Machine Learning for the decarbonisation of industry

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Abstract

Heavy industry requires high-temperature heat for many of its processes, which today is almost exclusively provided by burning fossil fuels. Many of those processes use the combustion of natural gas (methane) with air.

To reach a Net Zero Emission Scenario from combustion, the use of green fuels, such as hydrogen, ammonia, and eFuel is under consideration. The ability to easily switch to co-firing green fuel with hydrocarbon fuels or hydrocarbon fuels only would be a real advantage in facilitating their adoption, especially for hydrogen. Burning a blend of both fuels induces significant changes in combustion features while the process requirements must be guaranteed. The impact of such changes needs to be well understood. Therefore, new models and numerical approaches are needed for the assessment of blend combustion.

Objective

Co-firing hydrogen with hydrocarbon fuel :

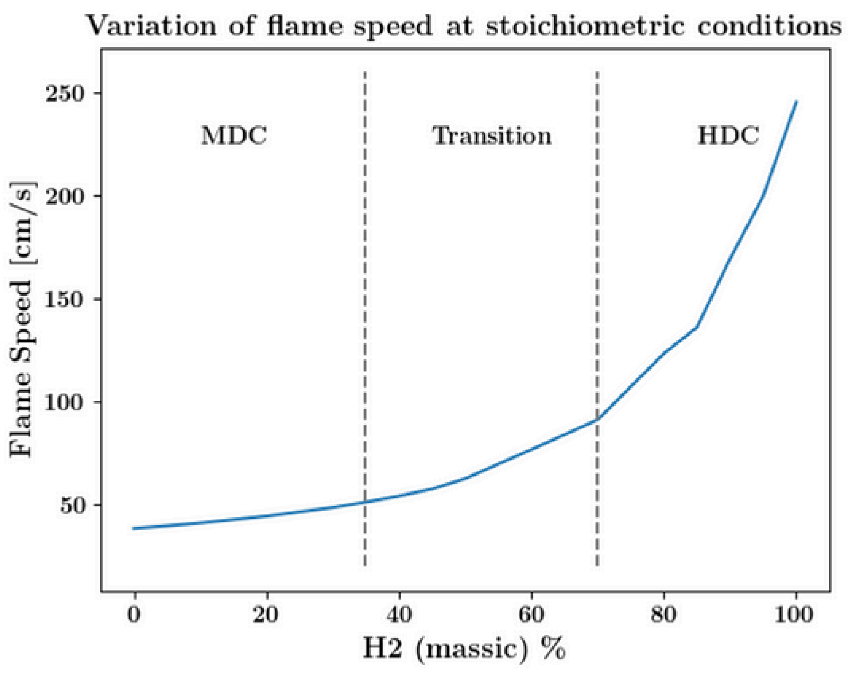
- **Flexibility:**
  - Overcome hydrogen supply variations and issues
  - Adapt to energy market prices
- **Sustainability:** Ensure limited pollutant emissions
- **Process:** Ensure the process is respected and product quality is conserved
- **Safety:** Certify the installations for infrastructures and workers

Challenges

Dual Fuel (CH4/H2) :

Burning a **blend changes thermochemical properties** like flame speed, length, overall temperature, and pollutant emissions.

Industrial furnaces are too big to be computed by direct numerical simulation, and experiments at scale are generally too expensive and limited in terms of measurements to characterize the flame.



There is a need for reduced models to deal with high-fidelity simulations of industrial combustion assets

Virtual Chemistry for Dual Fuel

Reference scheme (detailed chemistry) → **Learning database** (Equilibrium computations, 0-D reactors, 1-D flames, … — For every conditions of interest: $\phi, \beta, \Delta h, \ldots$) → **Optimization algorithm**

N_{sp}^v virtual species

N_r^v virtual reactions

$$\mathbf{X} = \begin{pmatrix} W_1 \\ a_{1,1} \\ a_{2,1} \\ \vdots \\ a_{5,N_{sp}^v} \\ a_{6,N_{sp}^v} \end{pmatrix}, \begin{pmatrix} A_1 \\ E_{a,1} \\ \vdots \\ A_{N_r^v} \\ E_{a,N_r^v} \end{pmatrix}$$

$$\text{Minimize } \mathscr{F}(\mathbf{X}) = \frac{1}{N_{cond}} \sum_{i=1}^{N_{cond}} \left(\frac{||\psi_i^{ref} - \psi_i^{opt}(\mathbf{X})||_{L_2}^2}{||\psi_i^{ref}||_{L_2}^2} \right)$$

with

$$\psi = (\bar{c}_p, \bar{h}, \overline{W}, T, S_L, \ldots)$$

Main virtual scheme[1]

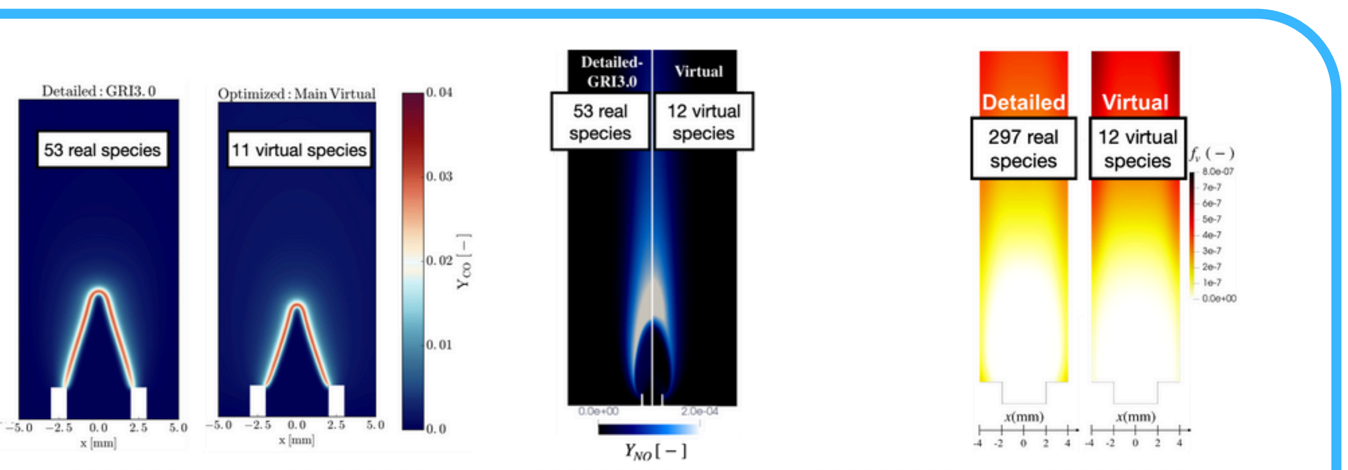
$$(1-\beta)\alpha_{F_1}F_1 + \beta\alpha_{F_2}F_2 + \alpha_{Ox}Ox \rightarrow \alpha_I I$$

$$\alpha_I I \rightarrow \sum_{k=1}^{N_P} \alpha_{P_k} P_k$$

- Heat release
- Temperature
- Laminar flame speed

+

Virtual satellite schemes



CO sub-scheme[2]

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

$$CO \leftrightarrow V_2$$

$$F + V_1 \rightarrow F + CO$$

- CO mass fraction

NO sub-scheme[3]

$$\alpha_F F + \alpha_{Ox}Ox \rightarrow \alpha_{V_1}^1 V_1 + \alpha_{V_2}^1 V_2 + \alpha_{V_3}^1 V_3$$

$$V_1 + F + Ox \rightarrow \alpha_{NO}^2 NO + \alpha_{V_2}^2 + F + Ox$$

$$F + NO \rightarrow F + V_2$$

$$V_3 \rightarrow NO$$

$$V_3 \rightarrow V_2$$

$$V_2 \leftrightarrow NO$$

- NO mass fraction

Soot sub-scheme[4]

$$\alpha_{F,1}^s F + \alpha_{Ox,1}^s Ox \rightarrow \alpha_{V_1,1}^s V_1 + \alpha_{V_3,1}^s V_3$$

$$V_1 \rightarrow \alpha_{\mathcal{S},2}^s \mathcal{S} + \alpha_{V_2,2}^s V_2$$

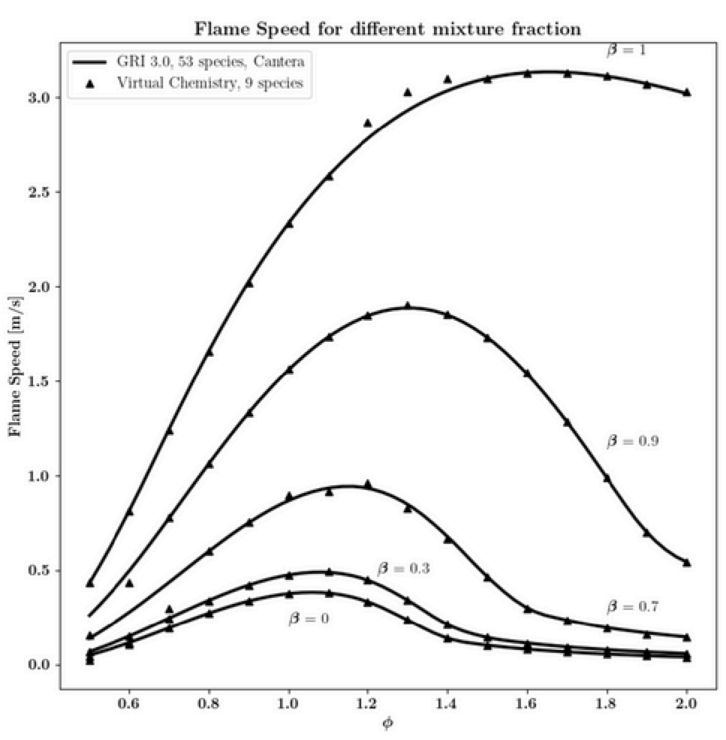
$$\mathcal{S} + V_1 + V_2 \rightarrow \alpha_{\mathcal{S},3}^s \mathcal{S} + \alpha_{V_3,3}^s V_3$$

$$\mathcal{S} + Ox + V_2 \rightarrow Ox + 2V_3$$

- Soot mass fraction

Results

A set of virtual products and reactions are identified to target the various conditions reached with detailed chemistry simulation



The thermodynamic properties of virtual products :

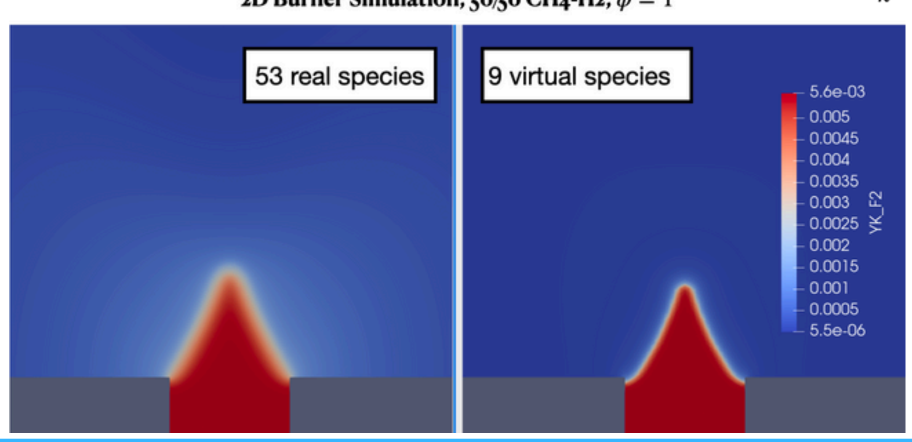
$$\frac{cp_k}{R} = a_{1k} + a_{2k}T + a_{3k}T^2 + a_{4k}T^3 + a_{5k}T^4,$$

Arrhenius law for Virtual mechanism:

$$k_{f_1} = A_1^v f_1^v exp\left(\frac{-E_{a,1}^v}{RT^v}\right) \prod_k^{N_{reactants1}} [\chi_k]^{\eta_{k,1}^v}$$

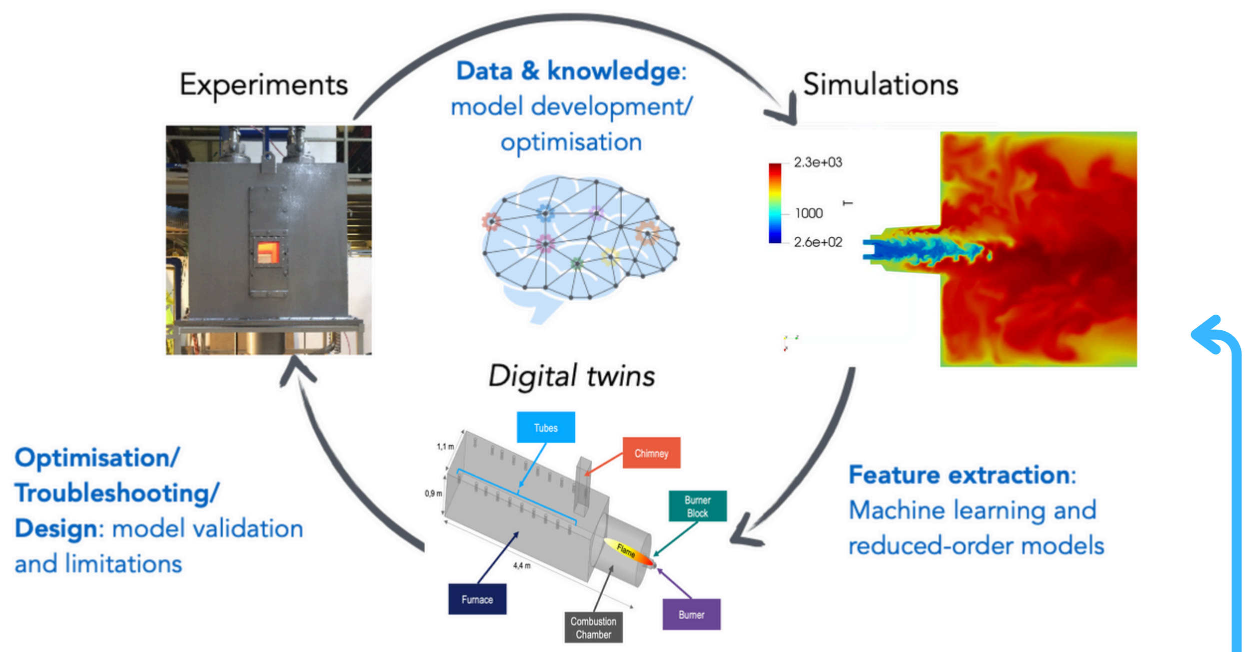
$$k_{f_2} = A_1^v f_1^v exp\left(\frac{-E_{a,1}^v}{RT^v}\right) \prod_k^{N_{reactants2}} [\chi_k]^{\eta_{k,2}^v}$$

2D Burner Simulation, 50/50 CH4-H2, $\phi = 1$



Future developments

Digital Twins [5]



Next Steps: Optimize all conditions and use interpolation to create virtual chemistry tables for dual fuel cases, enabling 2D validation simulations and subsequent 3D industrial applications.

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