Hydrogen and ammonia for industry decarbonisation
the role of diluted combustion technologies

Alessandro Parente

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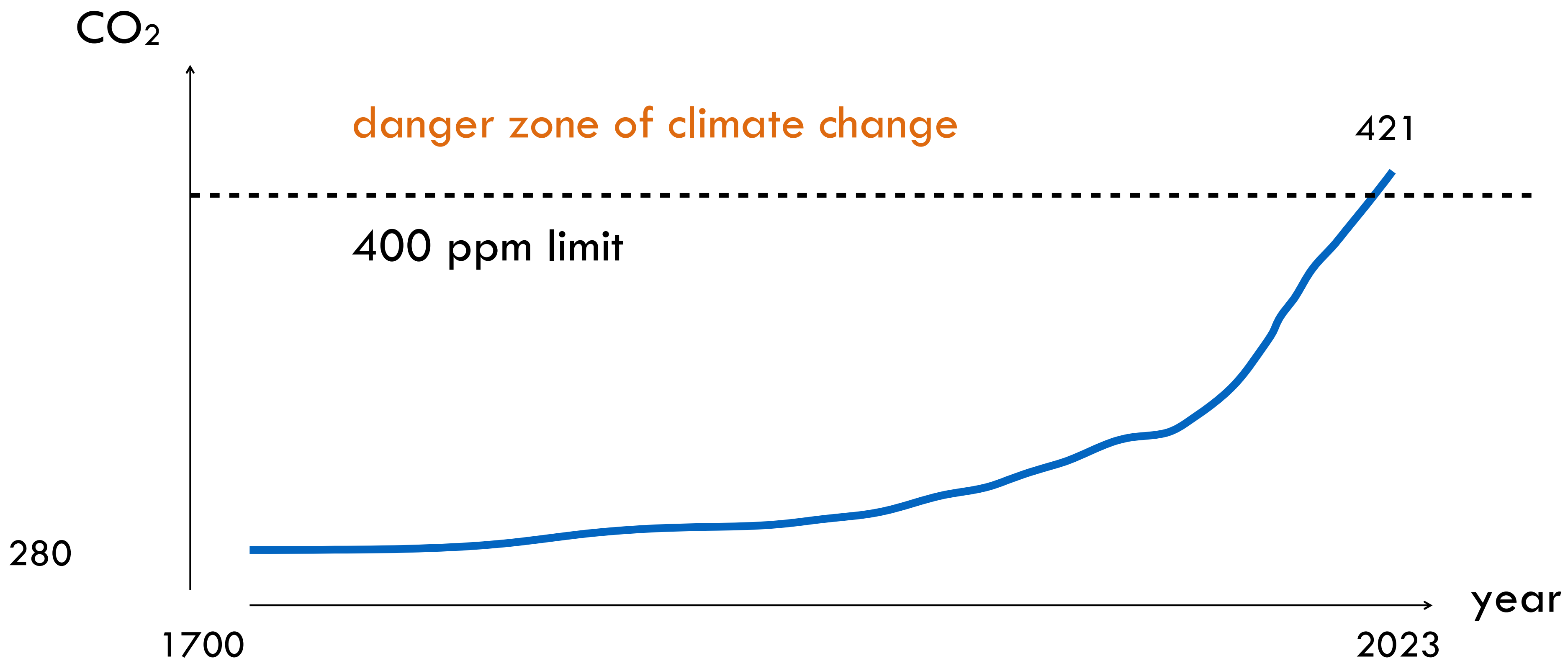
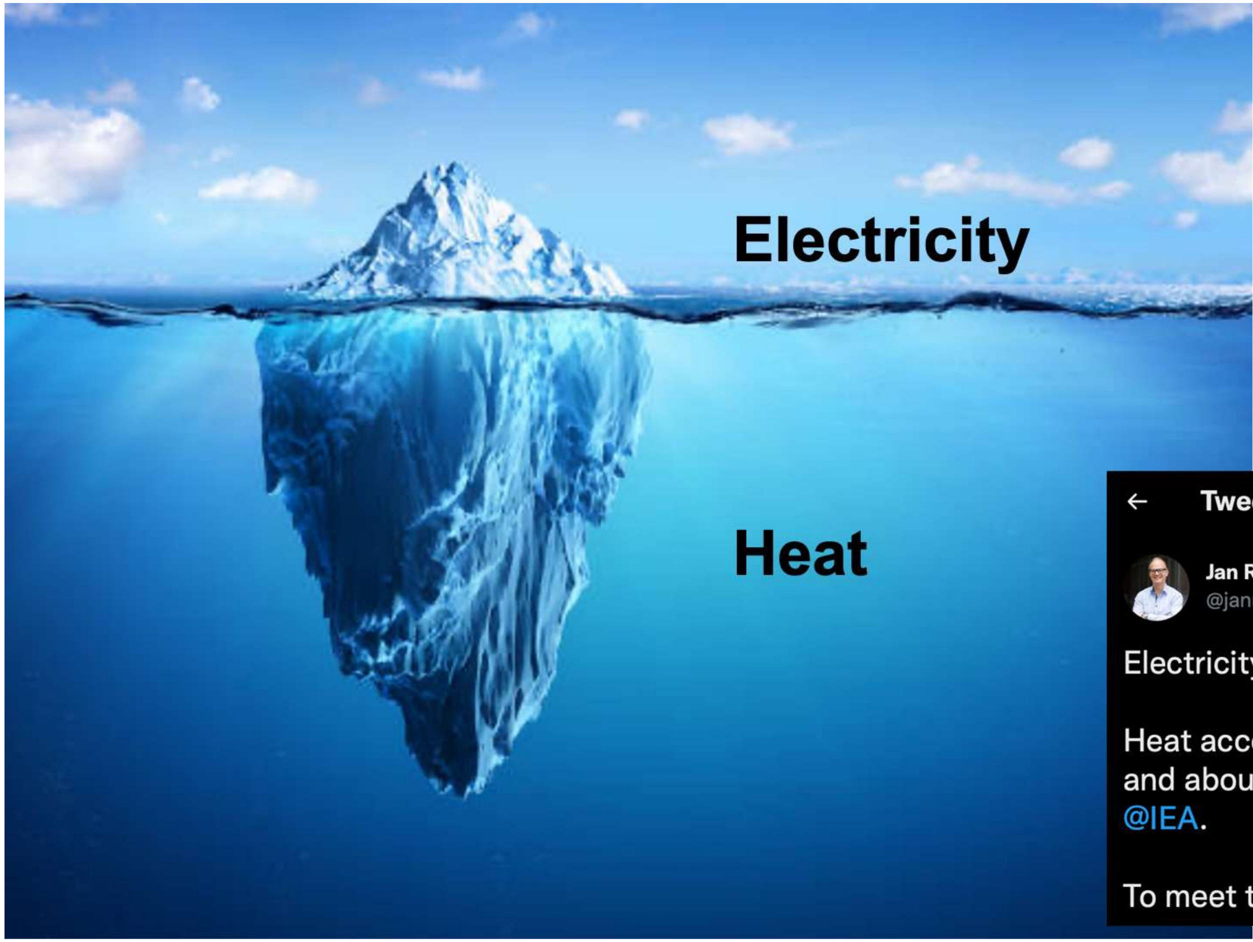
We have almost depleted our 'carbon budget' to limit a temperature increase of less than 1.5°C

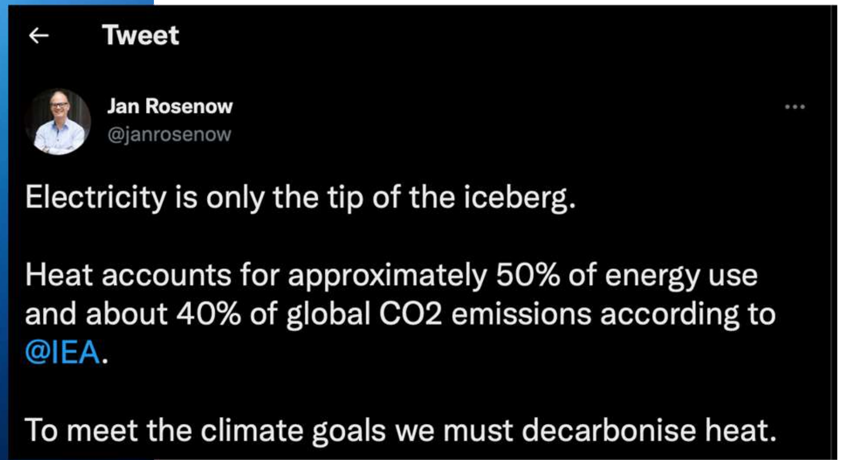


… and we're already suffering the consequences

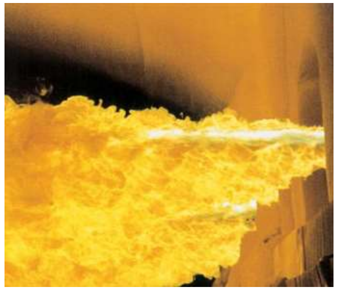
We have almost depleted our 'carbon budget' to limit a temperature increase of less than 1.5°C

Electricity is just the tip of the iceberg, the grand challenge is to decarbonise heat



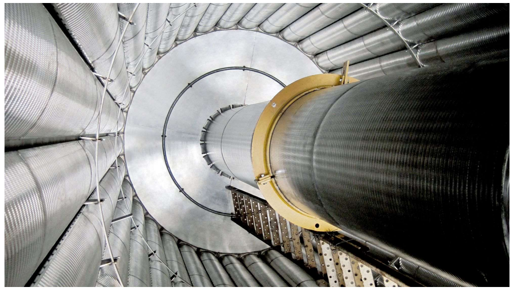


All sectors are equal, but some are more equal than others when it comes to net-zero targets: hard-to-abate sectors


High-temperature heat

Steel, glass, cement and aluminium



Non-energy sources

Ammonia and methanol



High-density, local energy sources

Shipping, trucking, aviation

The “elephant in the room” of the energy transition

“Around half of energy demand in energy-intensive industries is for high-grade process heat, which is challenging to electrify”

IEA World Energy Outlook 2022

In net-zero, hard-to-abate industries (HTAI) are a headache

30% of world's greenhouse gas emissions

10% of global CO_2 emissions from combustion processes for high-temperature heat

highly integrated and complex, needed in a net-zero world

Enablers for net-zero in HTAIs

Energy-efficiency improvements, energy savings and demand-size management

Optimisation, digitalisation and artificial intelligence

Further electrification of heat

Further electrification of processes

Use of climate-neutral hydrogen

CCUS

Sustainable biomass

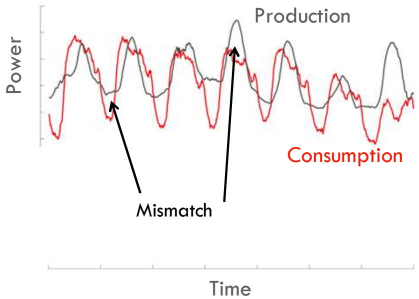
Improving circularity

Institute for EU studies report, 2018

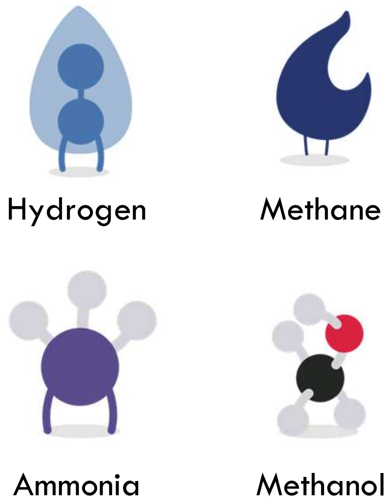
The excess energy from renewables can be transformed into renewable synthetic fuels

Excess of energy → Storage → Heat and electricity

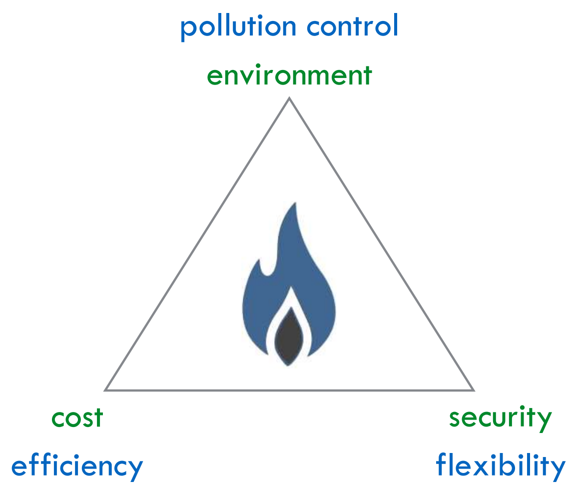
Renewables



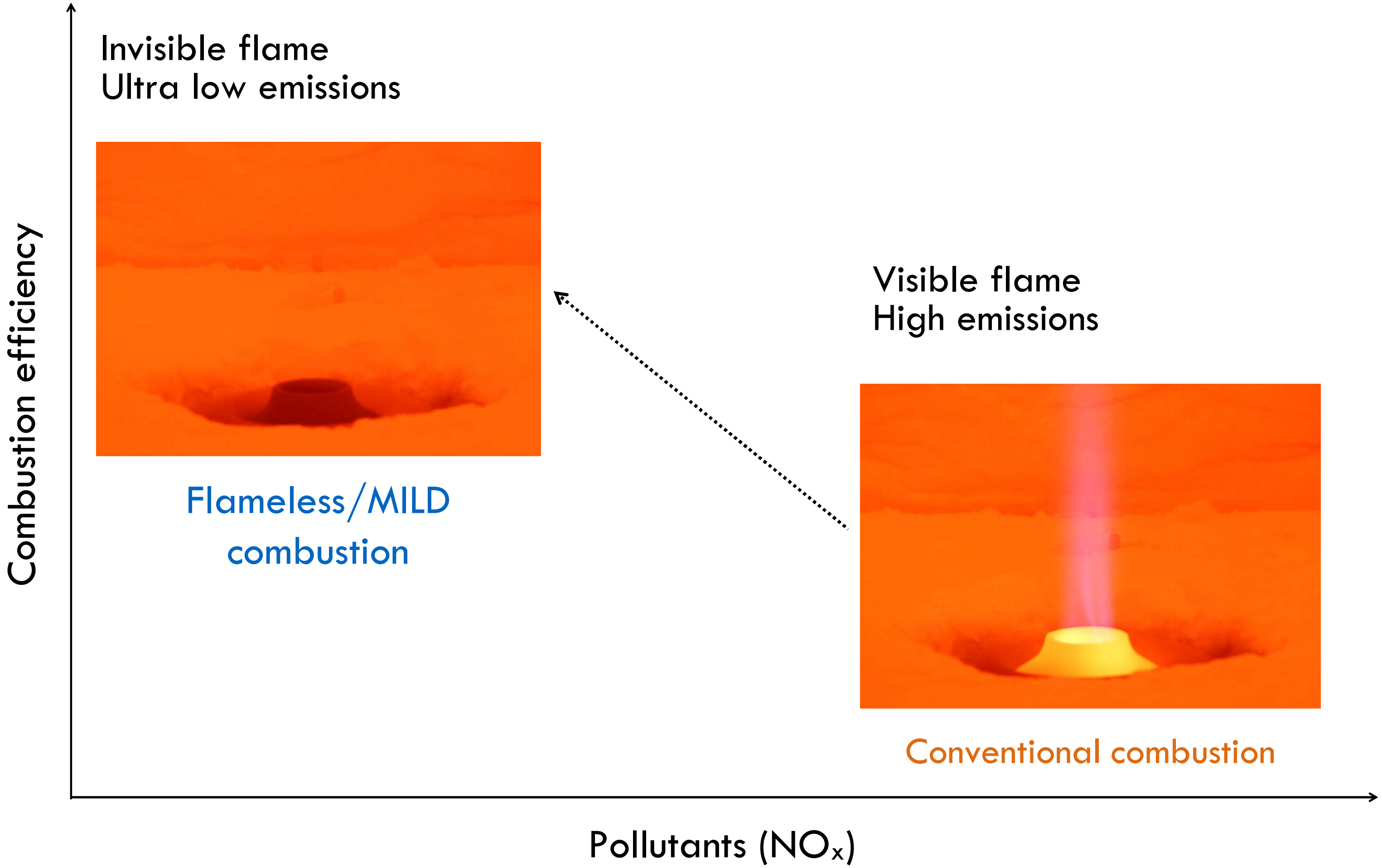
RSFs



New technologies



Flexible, efficient and clean technologies: sustainable combustion



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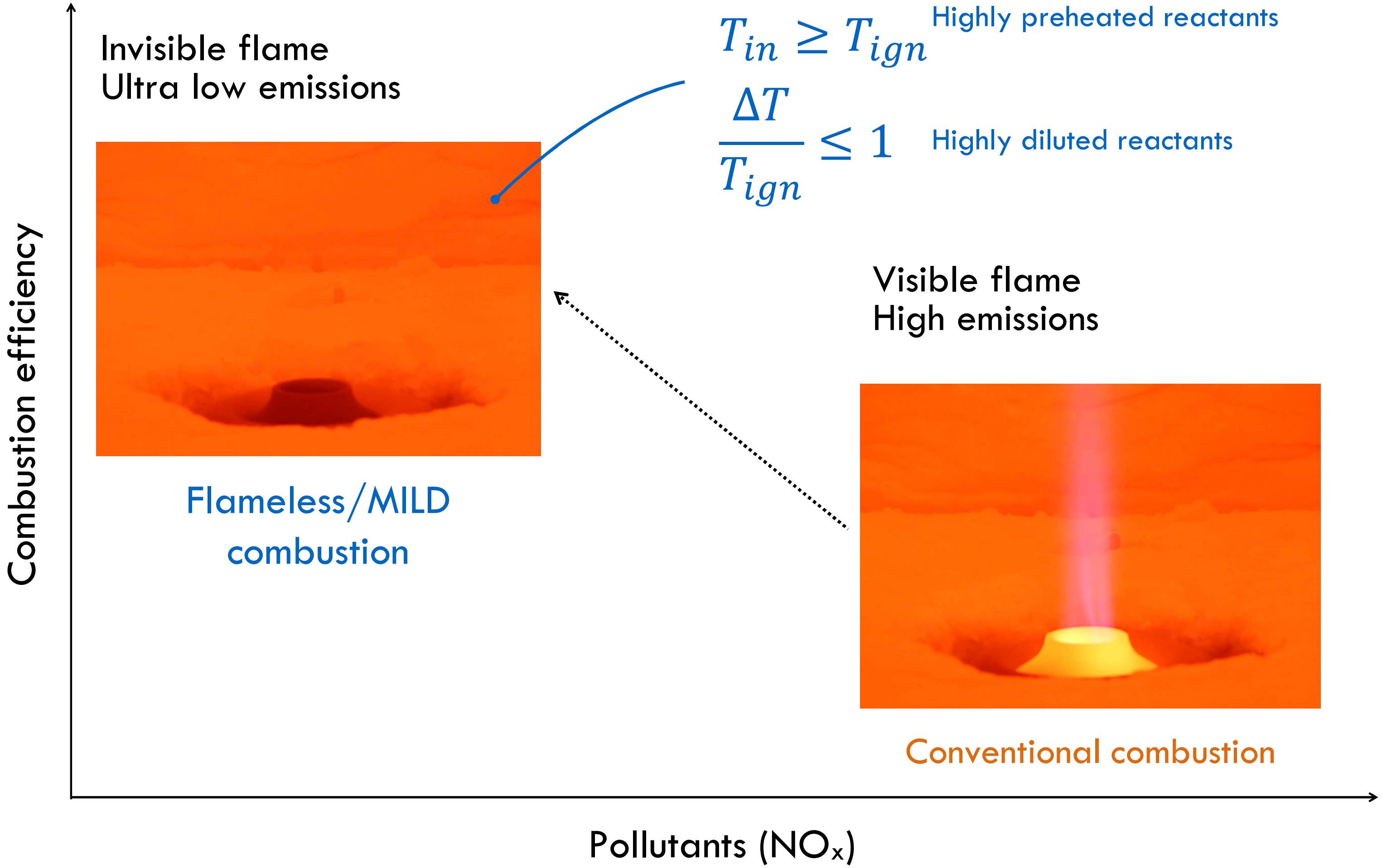
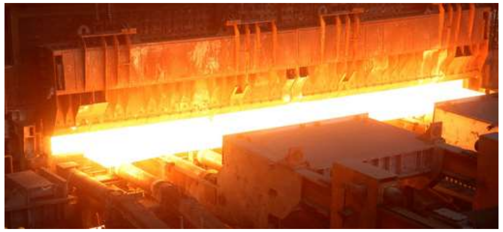


MILD features are appealing for a wide range of applications

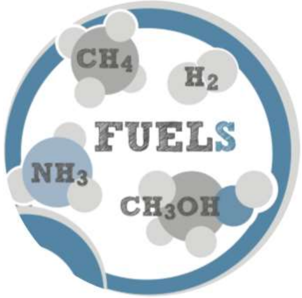
Uniform temperature

Heat treatments
Steel annealing
Glass making



Low pollutant emissions & high efficiency

Large fuel flexibility
Low-calorific value fuels
High-calorific wastes
H_2-enriched fuels
Oxy-fuel technologies

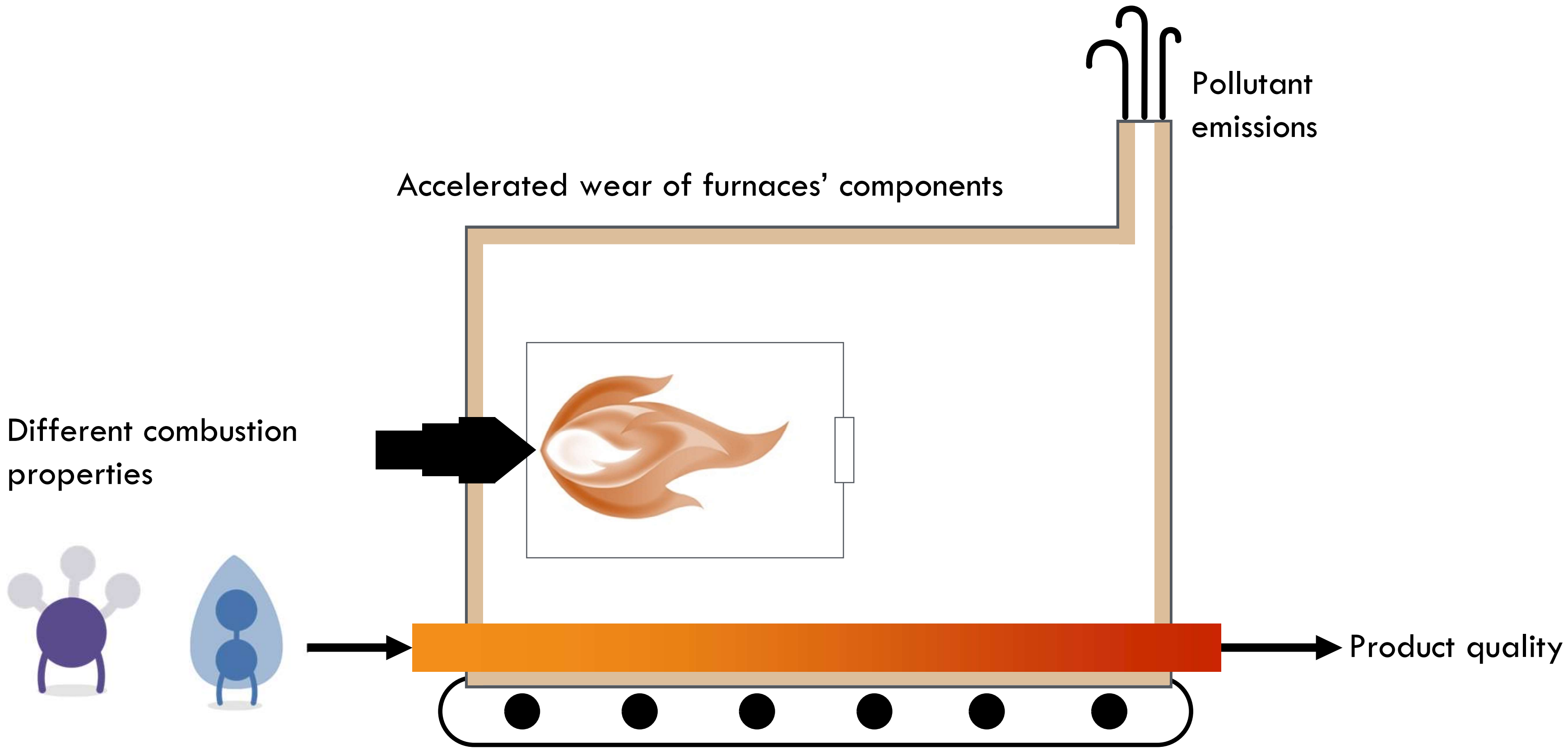


Noiseless (stable) operation

Gas turbines:
(GT and micro-GT)

www.dlr.de

Relying on RSFs raises a number of questions and technological challenges that remain to be answered



Ammonia and hydrogen show quite different combustion properties than traditional fuels

Ammonia

T_{ad}=2050 K

Methane

T_{ad}=2200 K

Hydrogen

T_{ad}=2380 K

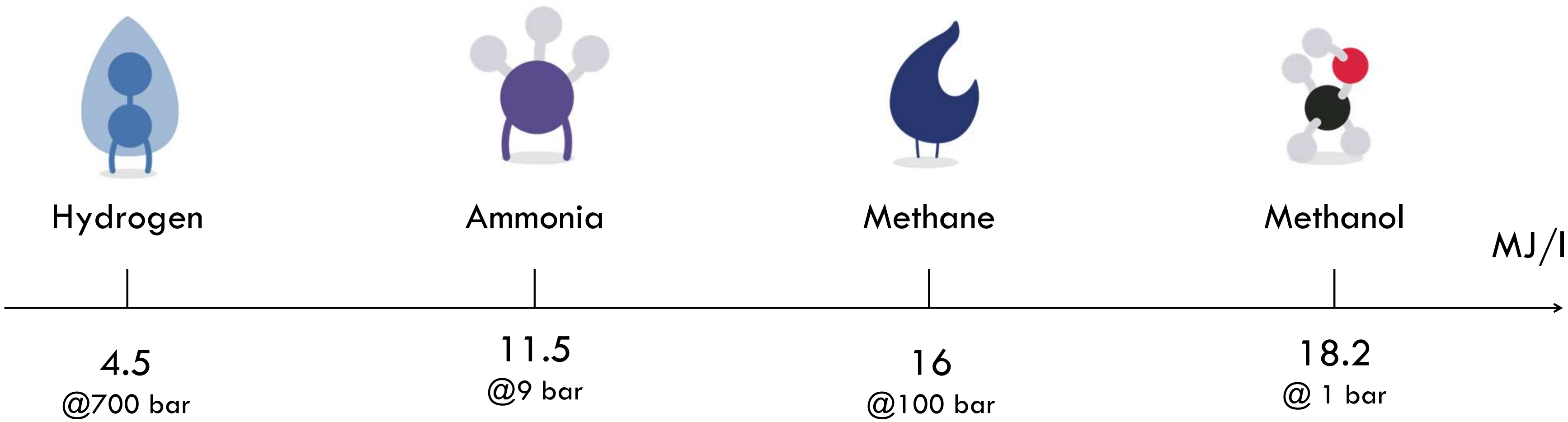
Ammonia and hydrogen show quite different combustion properties than traditional fuels

Ammonia	Methane	Hydrogen
		
T_{ad}=2050 K	T_{ad}=2200 K	T_{ad}=2380 K
S_L=0.07m/s	S_L=0.37m/s	**S_L=2.9m/s**

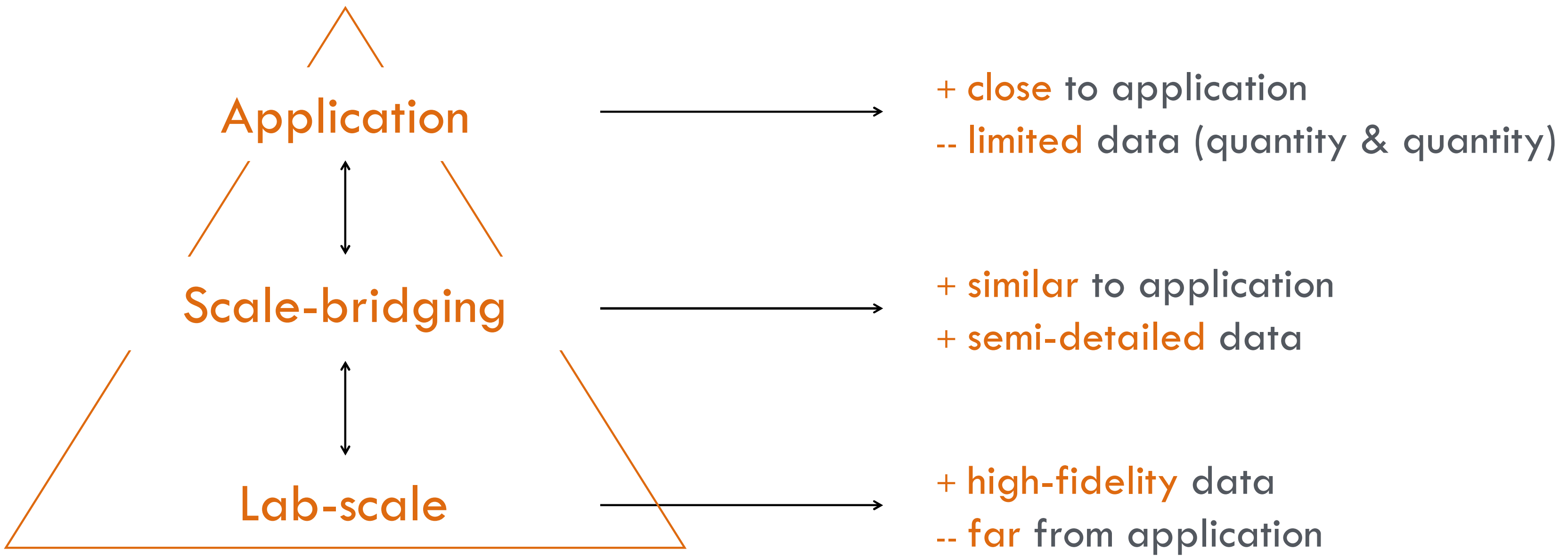
Ammonia and hydrogen show quite different combustion properties than traditional fuels

Ammonia	Methane	Hydrogen
		
T_{ad}=2050 K	T_{ad}=2200 K	T_{ad}=2380 K
S_L=0.07m/s	S_L=0.37m/s	S_L=2.9m/s
LHV=18.6 MJ/kg	LHV=50 MJ/kg	**LHV=120 MJ/kg**

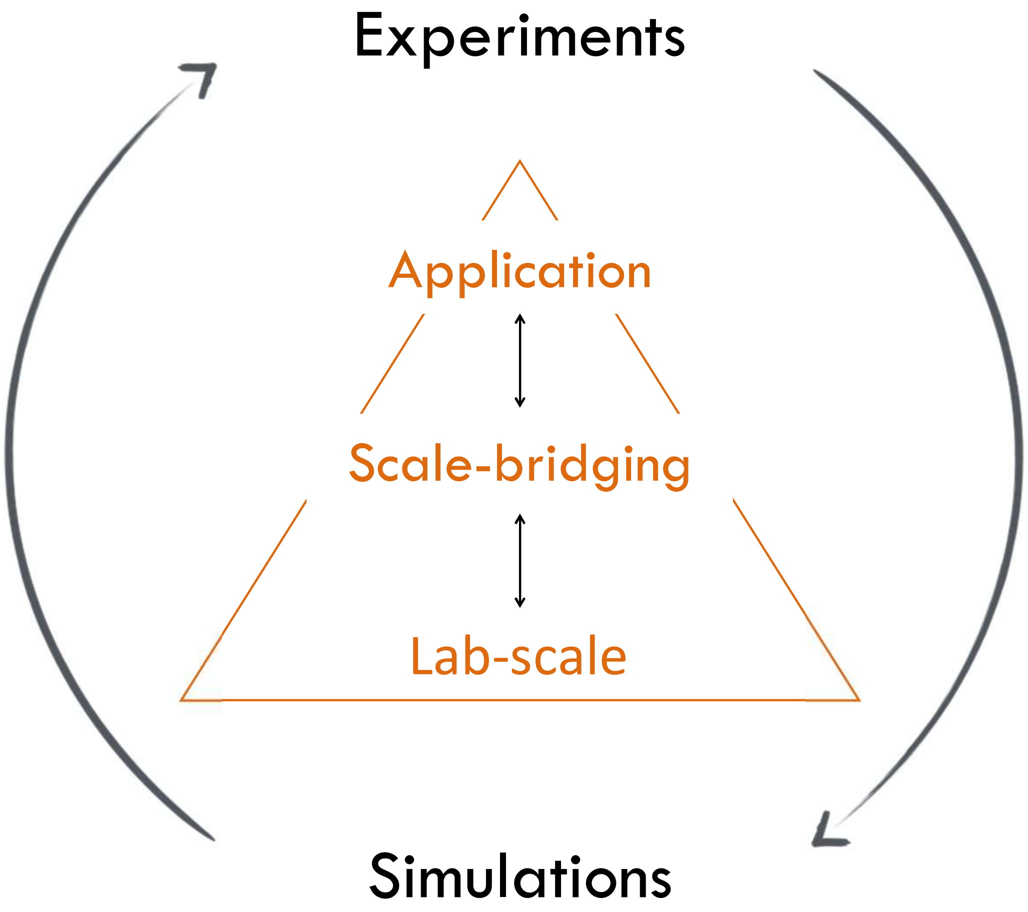
A palette of energy vectors with different volumetric energy densities



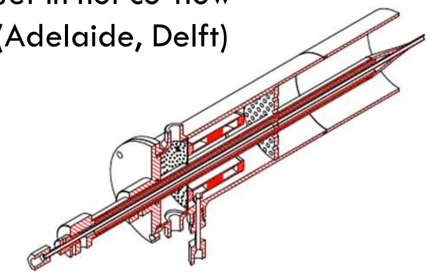
The scale at which information is available is also critical to take informed decisions

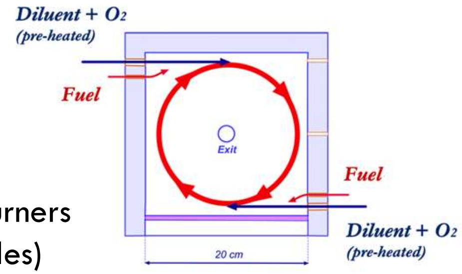


Validation hierarchies and scale-bridging data: flameless combustion

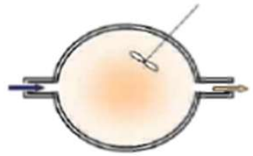


Jet in hot co-flow
(Adelaide, Delft)





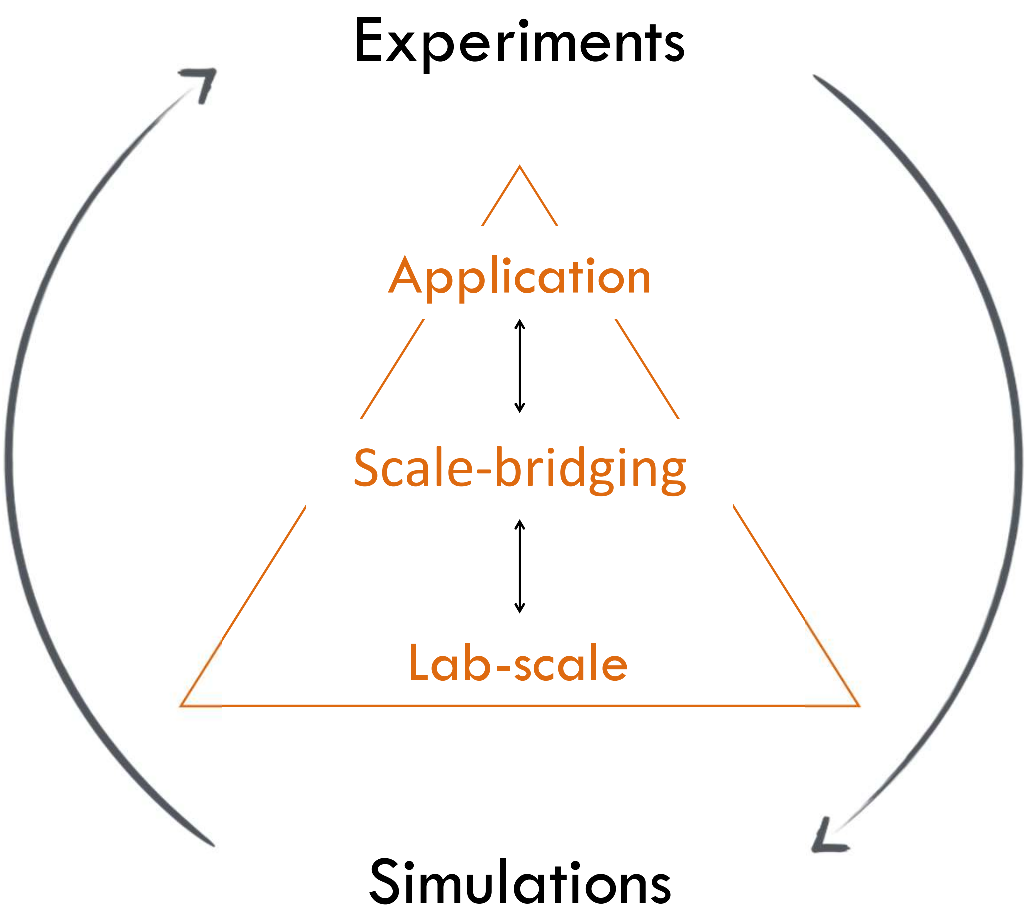
Cyclonic burners
(CNR, Naples)

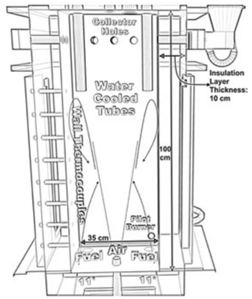


PSR experiments
(Orleans, Naples, …)

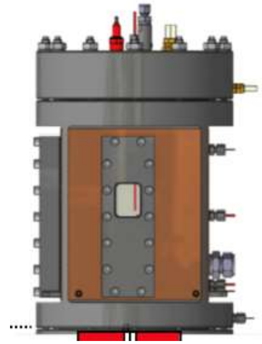
Validation hierarchies and scale-bridging data: combustion

MILD



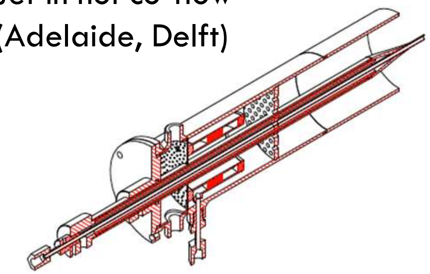


Lab-scale furnaces
(Delft, Mons)



Reverse-flow chambers
(Aachen, Brussels)

Jet in hot co-flow
(Adelaide, Delft)



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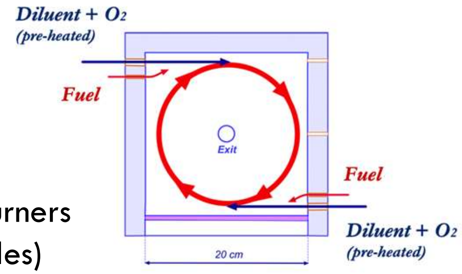

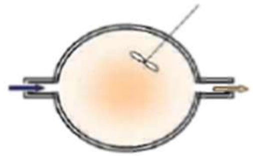

PSR experiments
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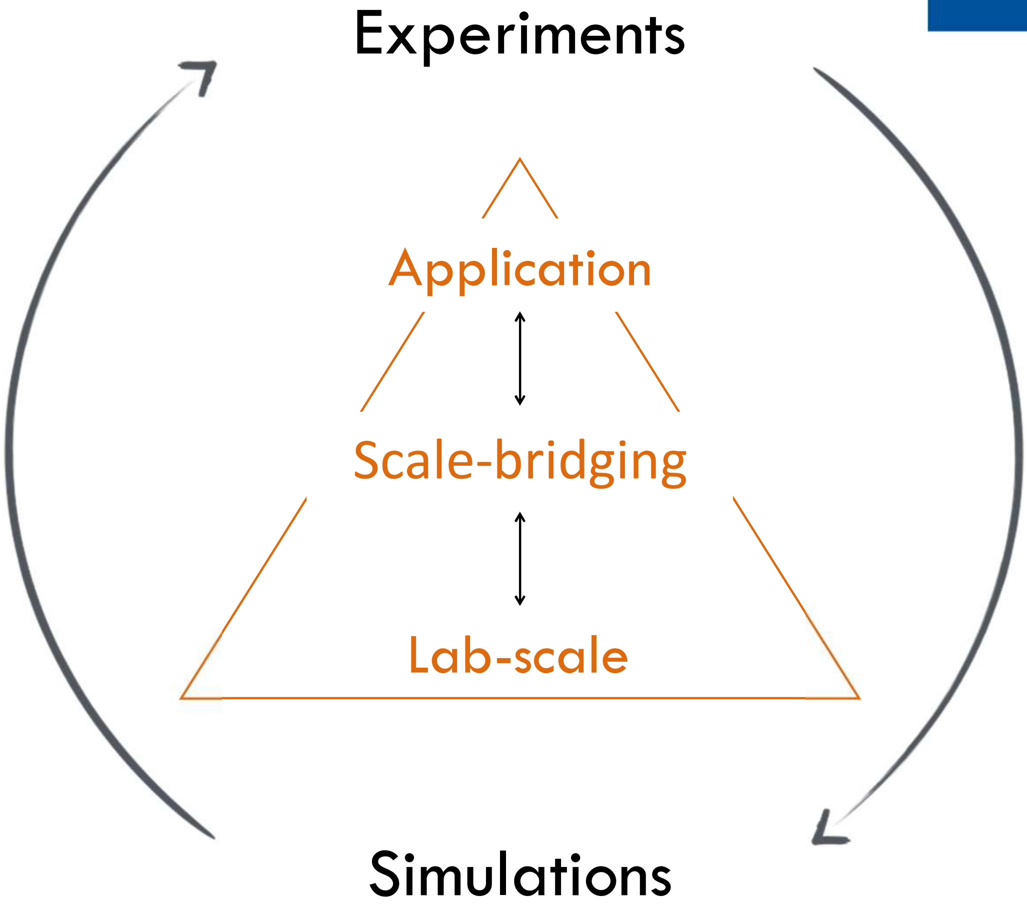
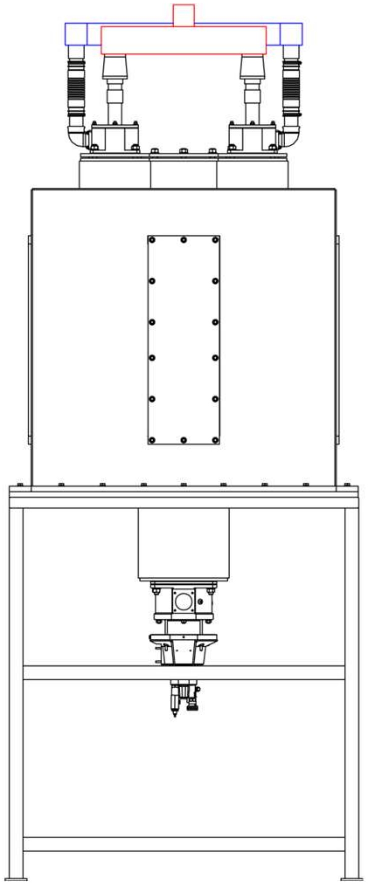


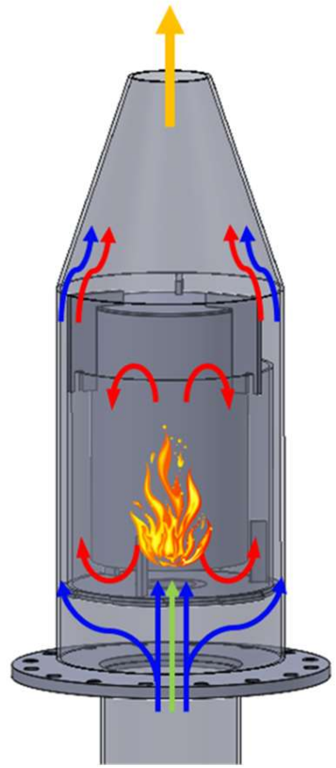
ULB

Furnace



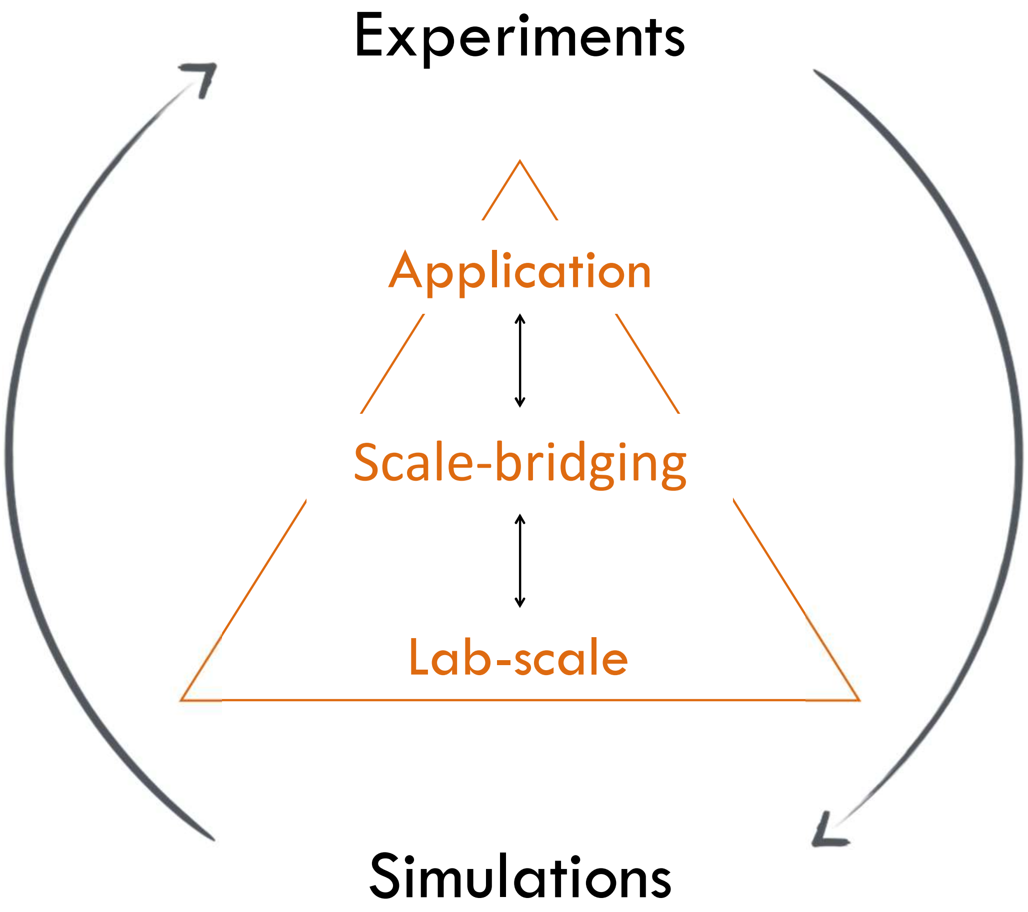
Built by WS

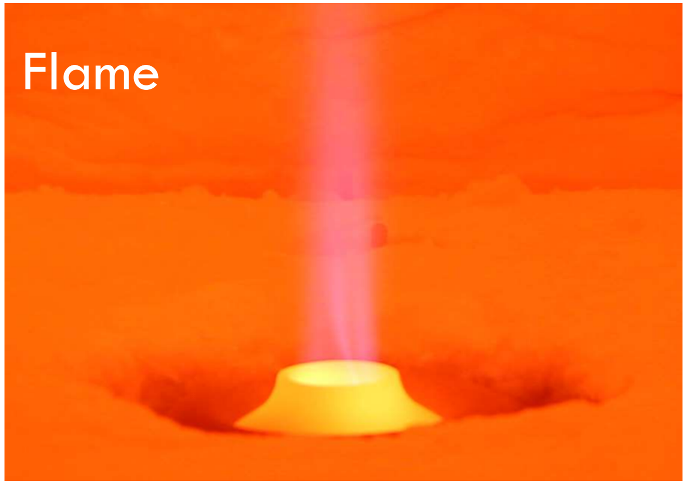
Stagnation-point
reverse-flow burner



Built by MITIS

Validation hierarchies and scale-bridging data: MILD combustion





Flameless should *always* refer to the combination

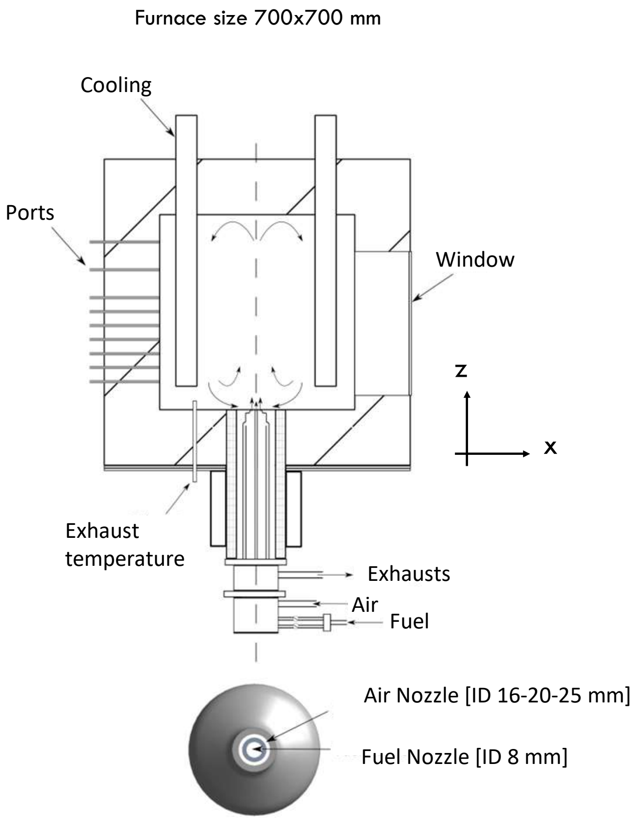
Fuel + burner + combustion chamber

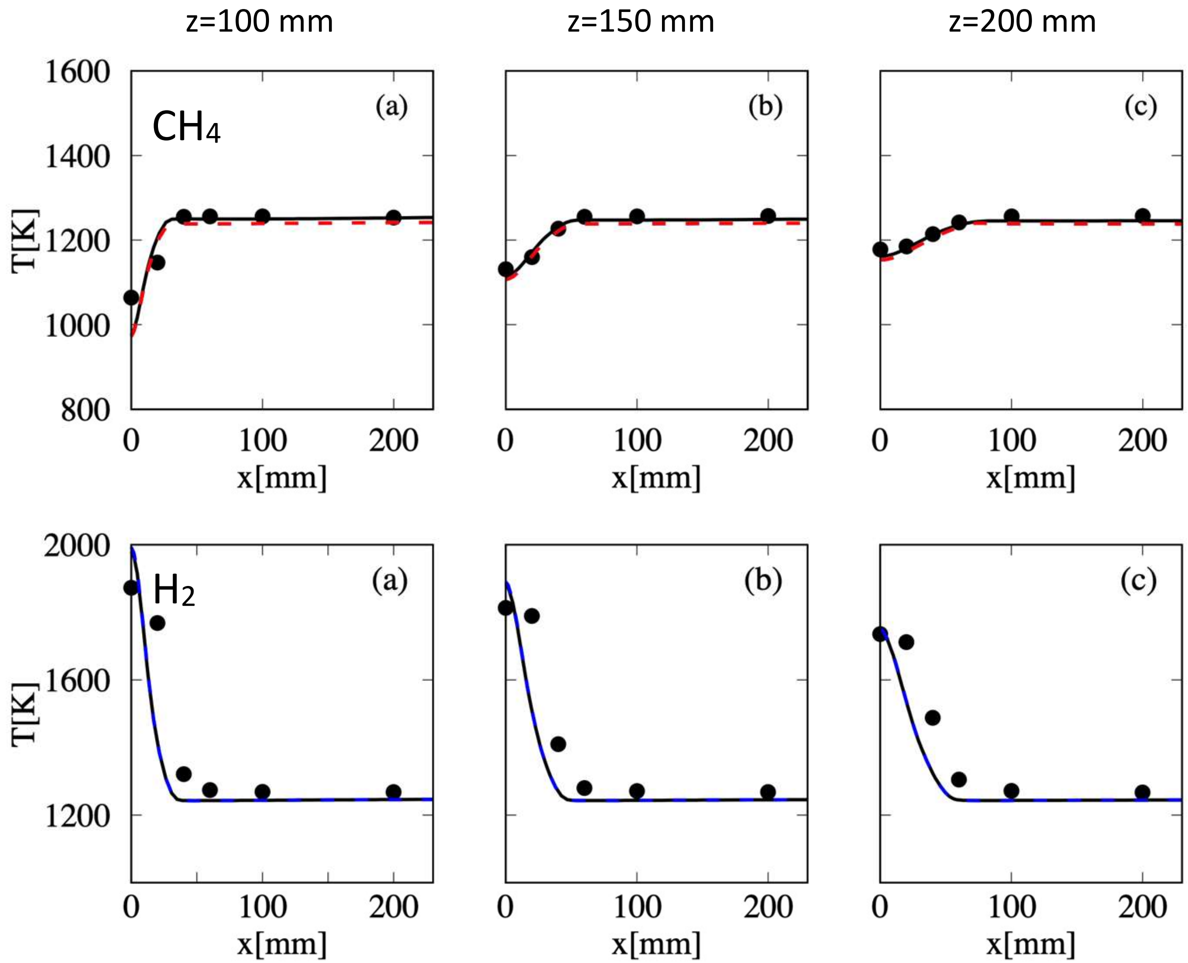
Determines the propensity to burning

Determines the mixing pattern

Constraints the exhausts' gas recirculation

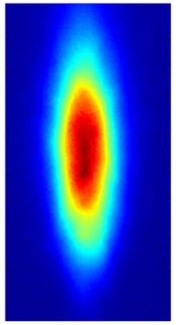
We performed experiments and simulations in a semi-industrial furnace fed with up to 100% hydrogen





Replacing methane with hydrogen results in a fundamentally different combustion behaviour

Methane



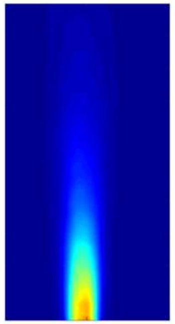
Low Da number

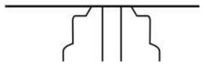
Chemistry controlled

Hydrogen

Mixing controlled

High Da Number





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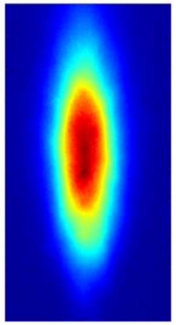

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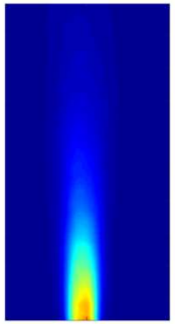
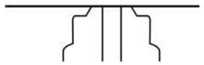
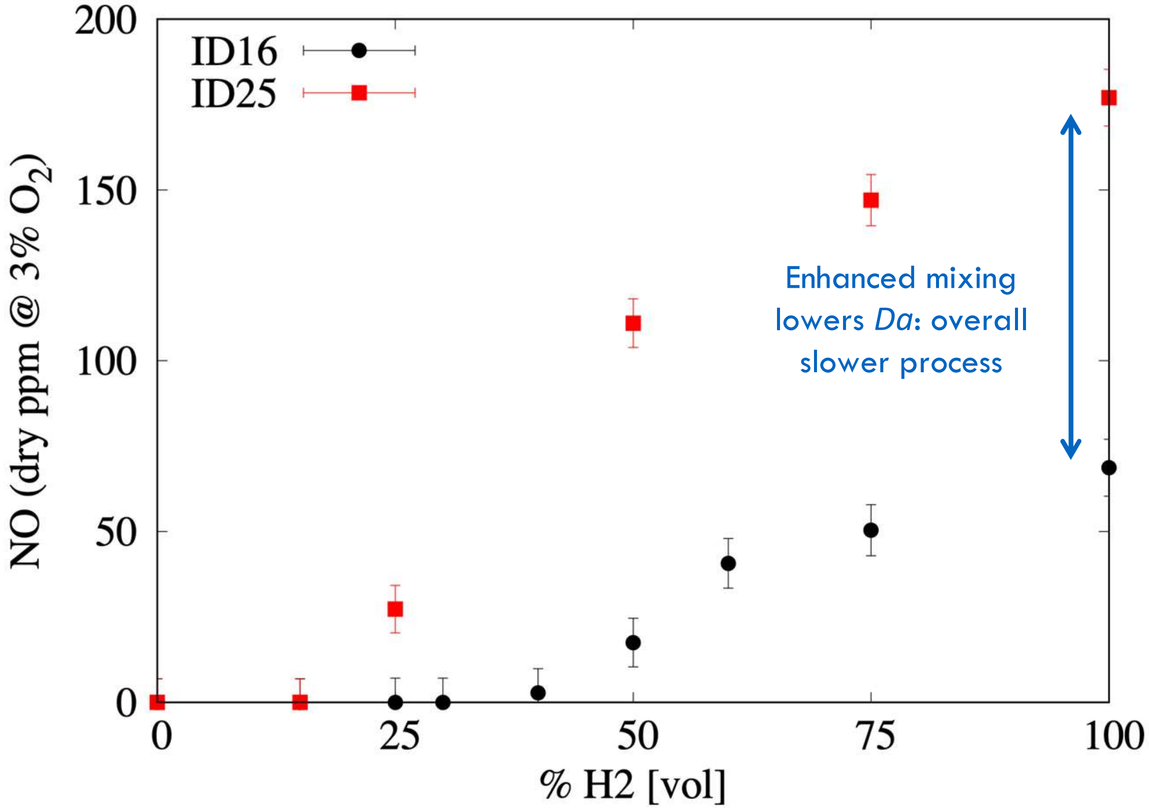
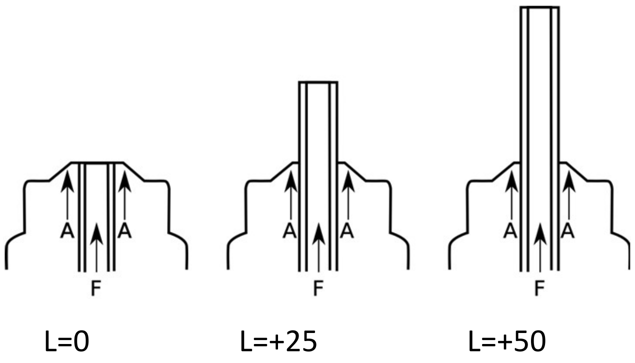


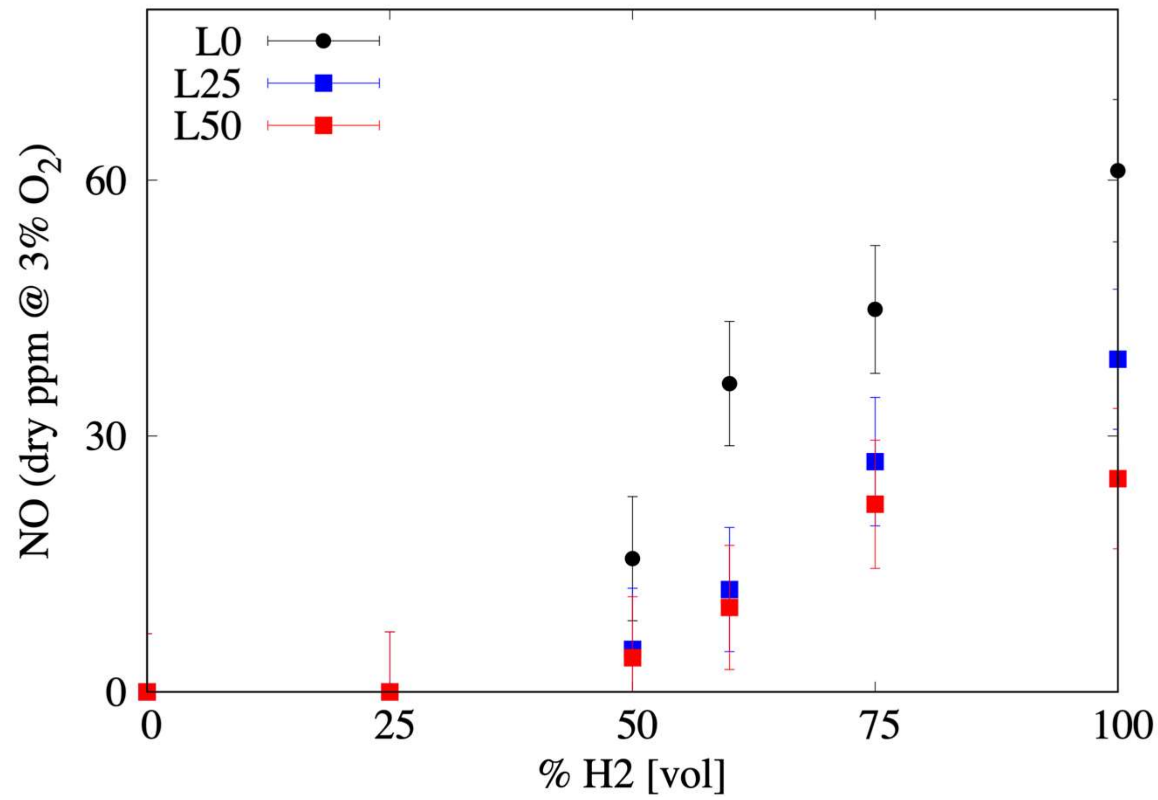




A design modification was required to promote mixing between exhaust and air before combustion, and lower NO_x



Ferrarotti et al., IJHE (2021)



We investigated the feasibility of pure ammonia combustion under conventional and flameless combustion

Narrow flammability limits
Low flame speeds
Low adiabatic flame temperature
High NO_x (N bonded to the fuel)

→

Resorting to reactivity enhancers (oxy, H_2)
Partial or total NH_3 cracking
Staged combustion

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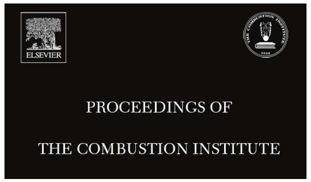
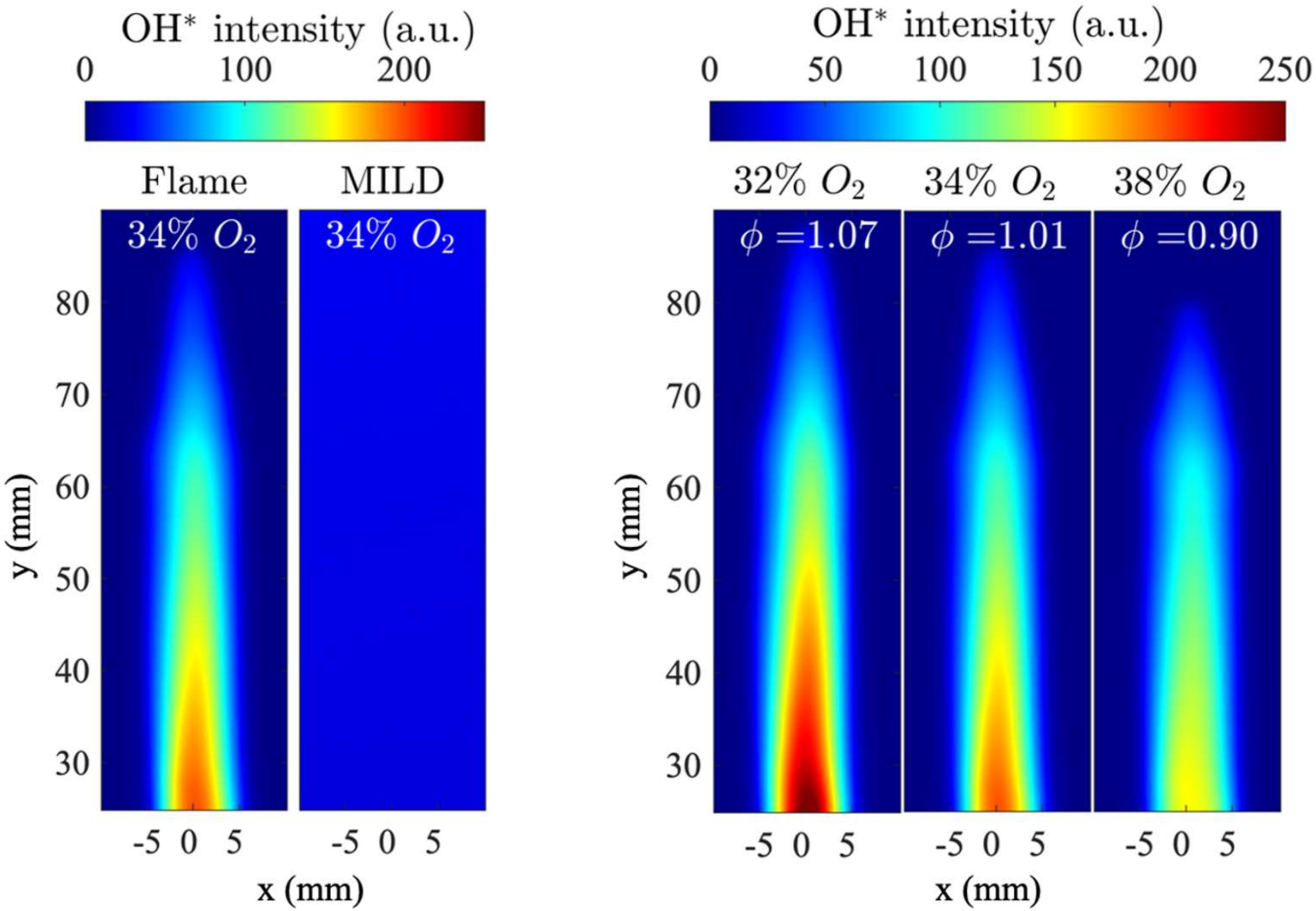


M. Cafiero, S. Sharma, M.M. Kamal, M.L. Lavadera, S. Iavarone, A. Coussement, A. Parente
Enhancing Pure NH_3 Combustion: Impacts of O_2 Enrichment under MILD Conditions in a 20-kW Semi-industrial Scale Furnace
Proceedings of the Combustion Institute, 40, 2024, 105336

We performed an extensive campaign to assess the emission characteristics of ammonia combustion in MILD conditions

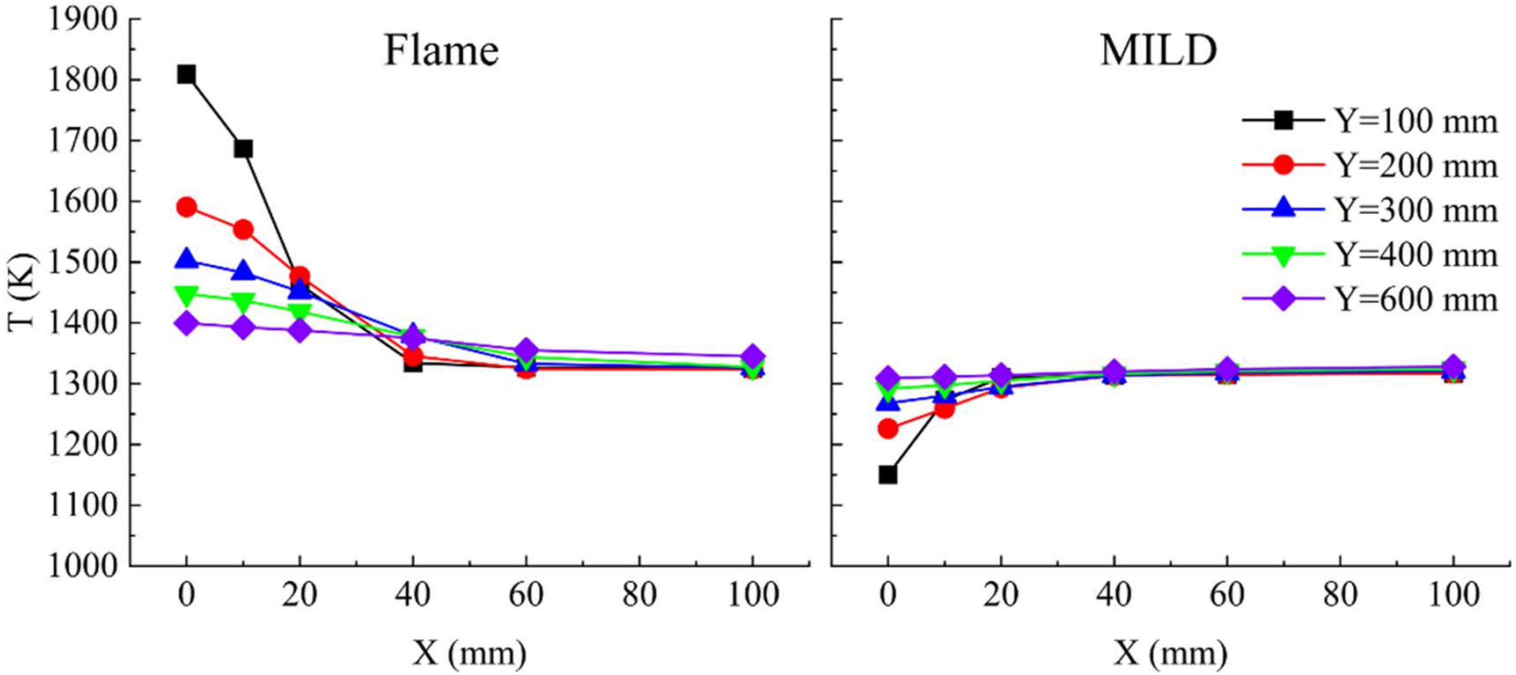
Parameter	MILD mode		Flame mode
Oxidizer injector	(ID16)	(ID20)	(ID16)
Thermal input (kW)	20	20	20
Cooling air, $\dot{Q}$ (Nm^3/h)	8.3-16.3	16.3	16.3
Oxidizer, $\dot{m}$ (kg/s)	$2.82\ x\ 10^{-3} – 5.48\ x\ 10^{-3}$	$4.07\ x\ 10^{-3}$	$4.07\ x\ 10^{-3}$
NH_3, $\dot{m}$ (kg/s)	$1.08 \cdot 10^{-3}$	$1.08 \cdot 10^{-3}$	$1.08 \cdot 10^{-3}$
ϕ (-)	0.70-1.6	0.70-1.6	0.70-1.6
O_2 (%)	21-50	21-50	21-38
O_2/N_2 ratio	0.27-1	0.27-1	0.27-0.92

Stable ammonia combustion was achieved at a minimum O_2 enrichment of 30% in conventional conditions and 34% in MILD mode

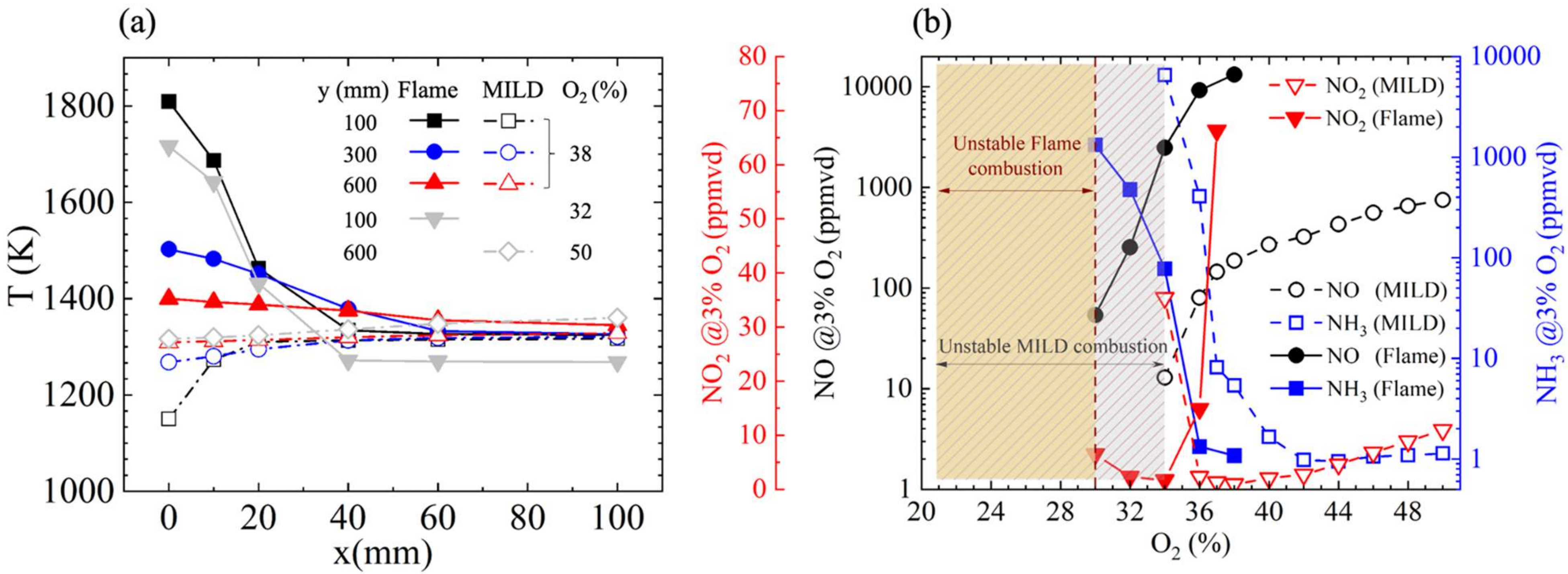


More distributed combustion and overall temperature reduction was observed in MILD conditions

O_2 enrichment = 38%



For the same O_2 enrichment, NOx emissions are higher in flame mode than in MILD



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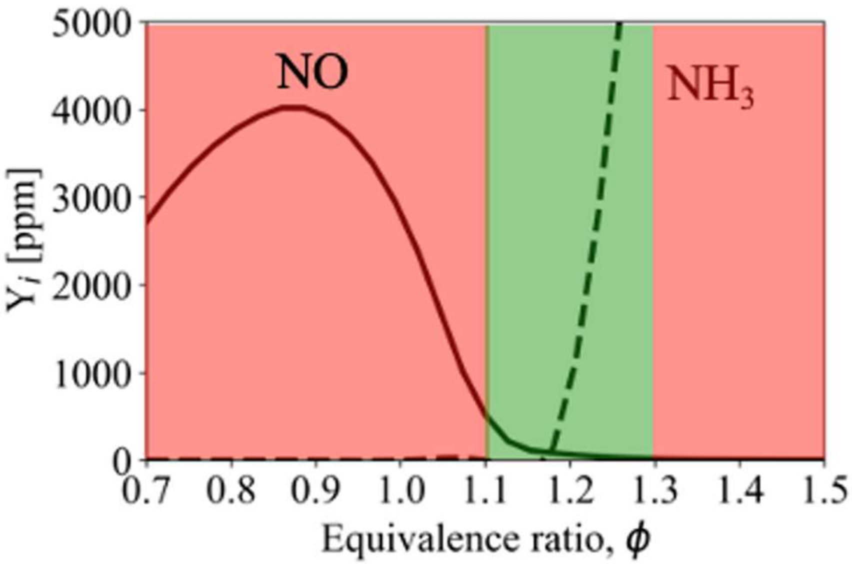

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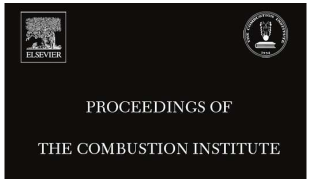
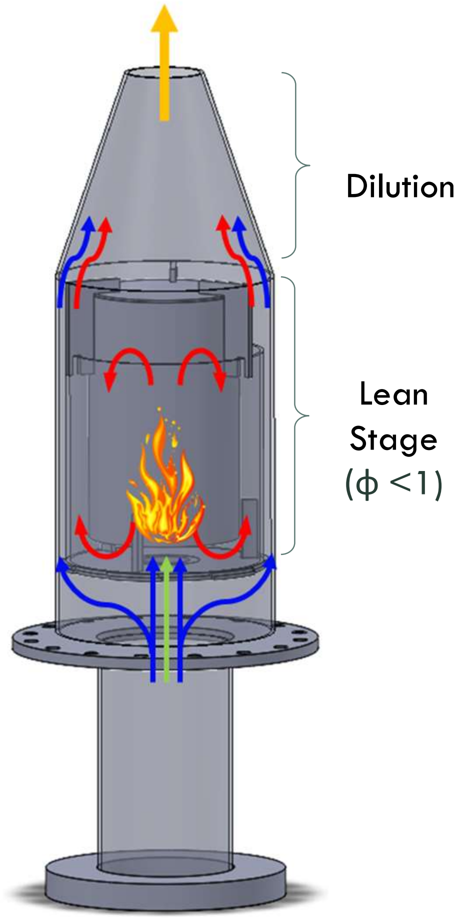
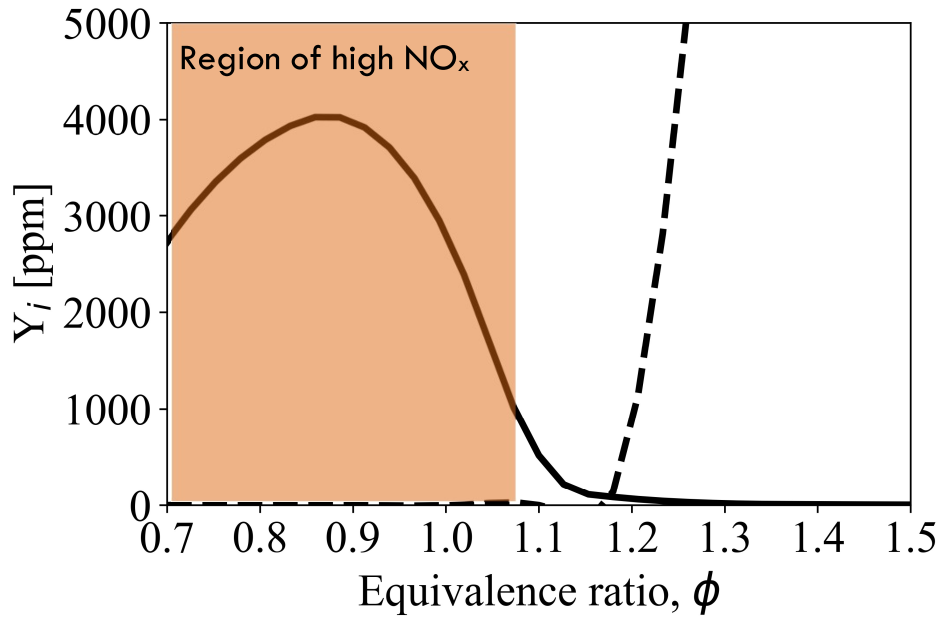


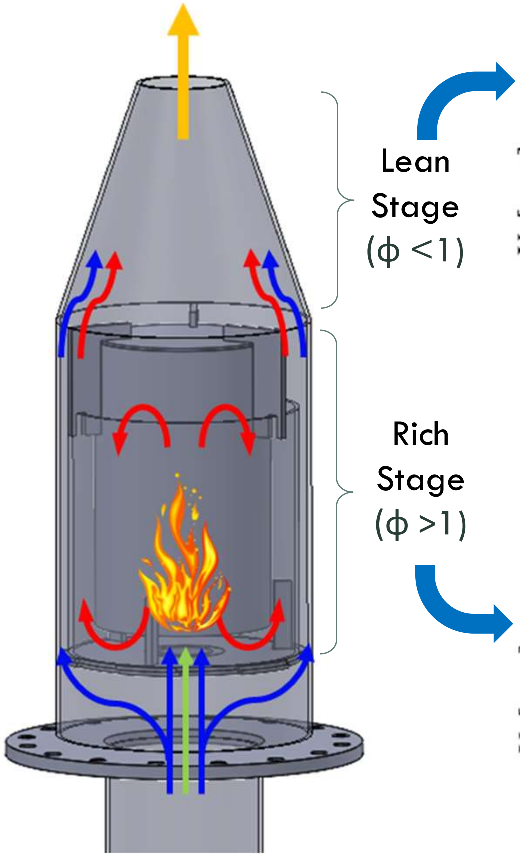
Lorenzo Giuntini, Chiara Novelli, M. Mustafa Kamal, Marianna Cafiero, Chiara Galletti, Axel Coussement, Alessandro Parente
Continuously-staged NH oxidation in a stagnation-point reverse-flow combustor for low NO emissions
Proceedings of the Combustion Institute, 40, 2024, 105674

We investigated the feasibility of staged ammonia combustion in the two-stage design by MITIS (for CH_4)

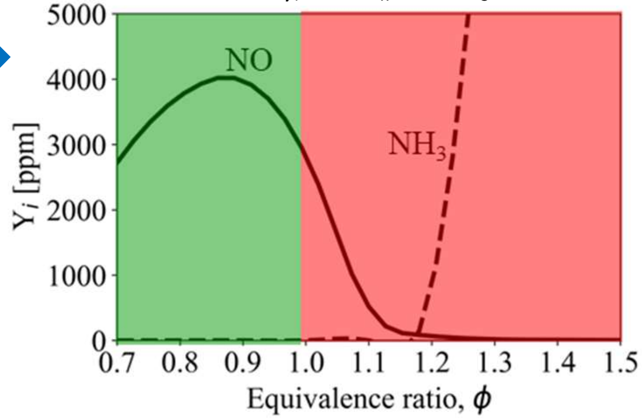




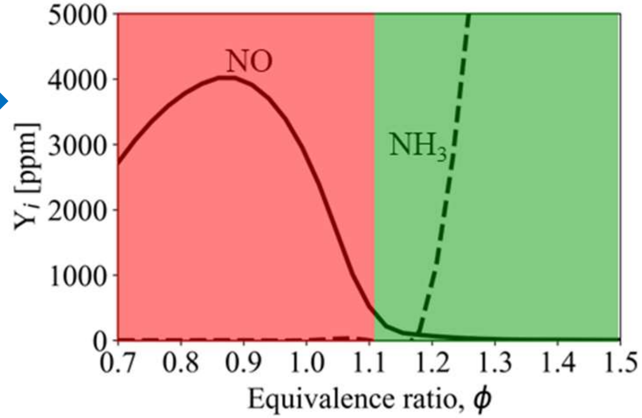
A solution is to adjust the injectors and flow rates to perform a rich-quench-lean (continuous) sequence



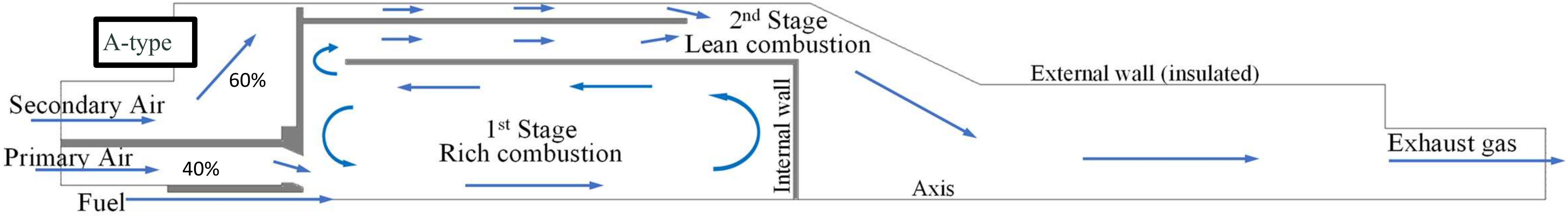
Ideally, no NO_x and NH_3



Some NO_x and unburned NH_3

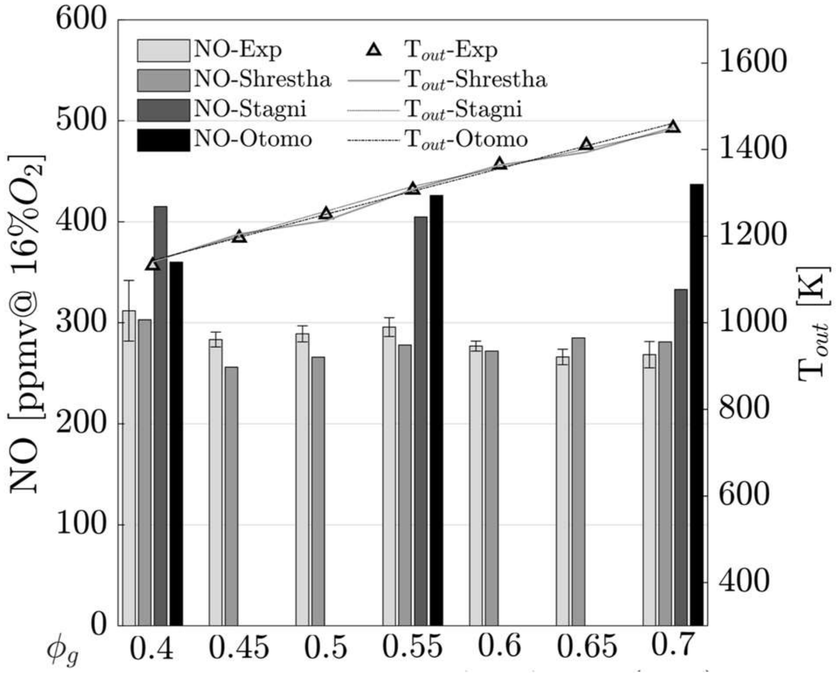


We empty the baseline configuration to develop and validate a numerical model



- 2D Steady state RANS simulations
- Turbulence model : Realizable k-ε
- Combustion model: PaSR with C_{mix}=0.1
- Kinetics: Otomo [1], Stagni [2], Shrestha [3]

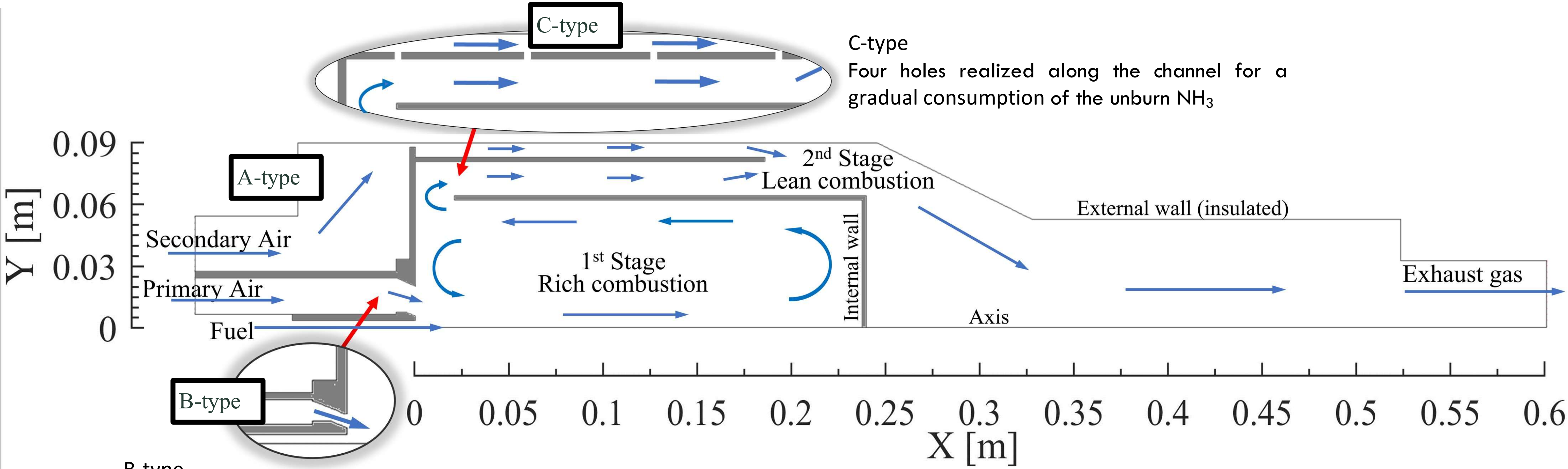
T_{in}=300K, p=1 bar, φ_1=1-1.7



[1] Otomo et al., IJHE 43 (2018) 3004-3014 [2] Stagni et al, CEJ 471 (2023) 144577 [3] Shrestha et al, PROCI 38 (2021) 2163-2174

Two additional designs were developed for virtual prototyping

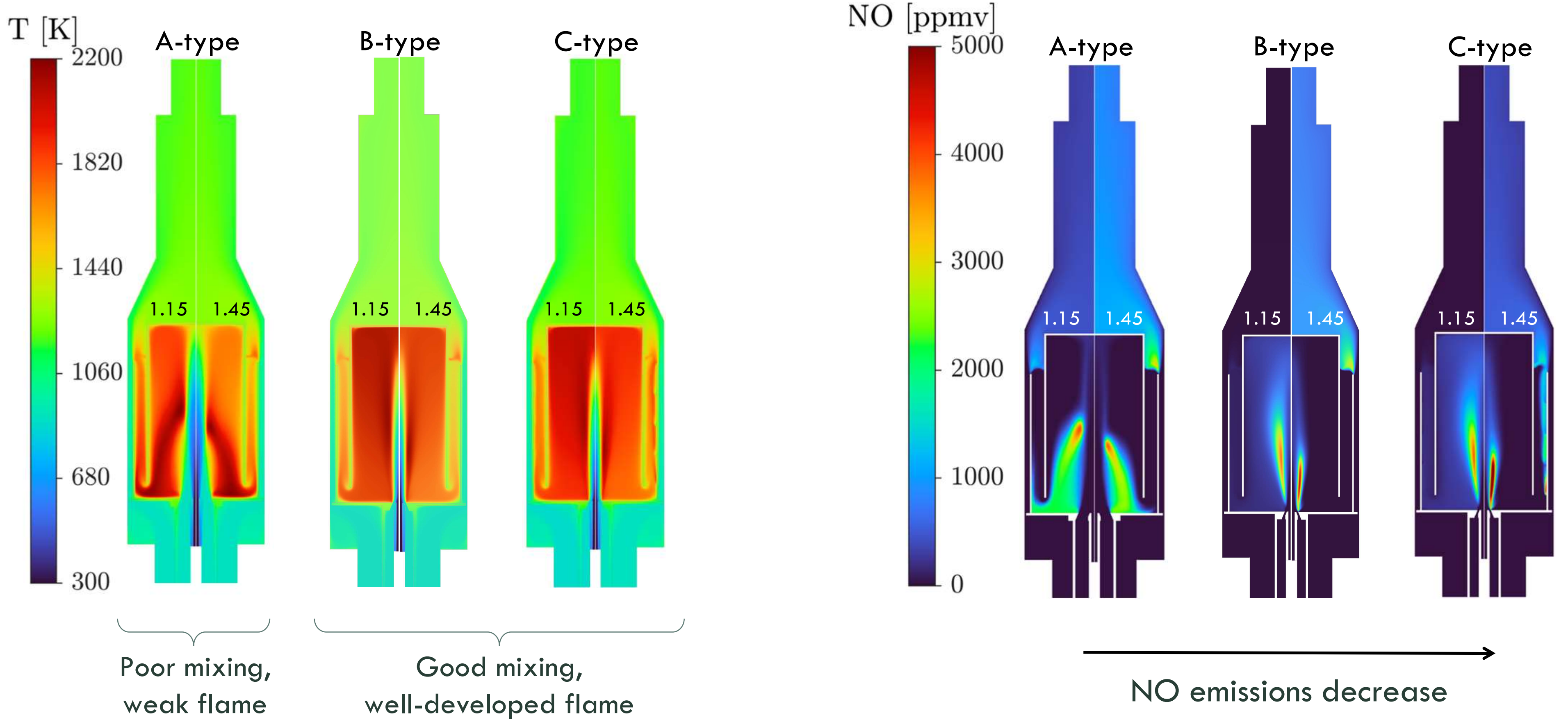
T_{in}=900K, p=1 bar, φ_1=1.15-1.45



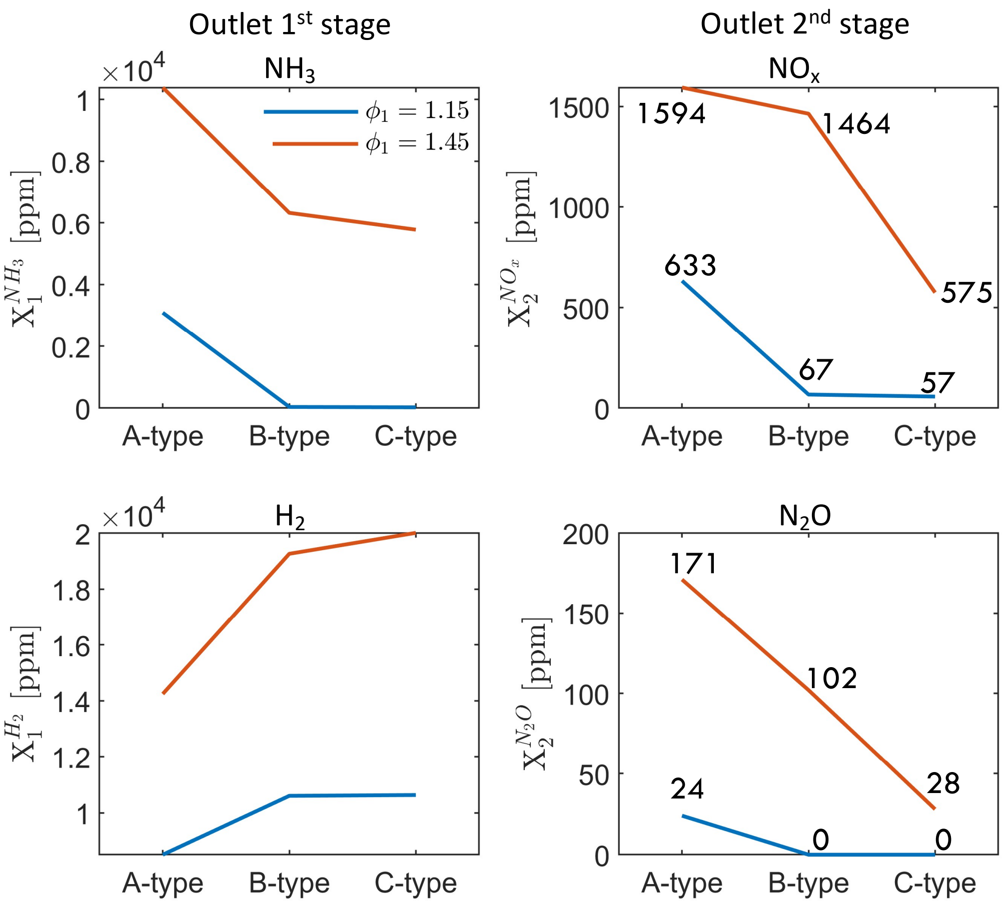
C-type
Four holes realized along the channel for a gradual consumption of the unburn NH_3

B-type
The Primary Air nozzle diameter is reduced to improve mixing in the 1st stage

The continuous staging design ensures high combustion efficiencies and low emissions



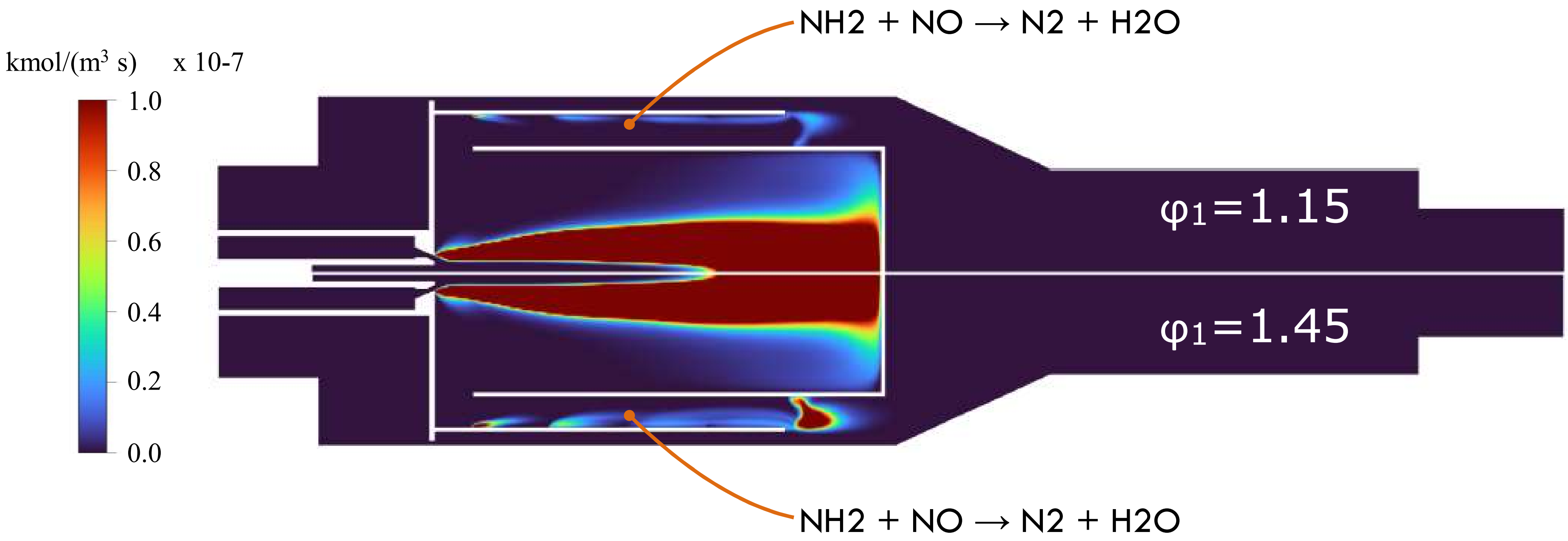
A 90% NO_x emission reduction was observed from the base design to continuous staging, with no ammonia slip



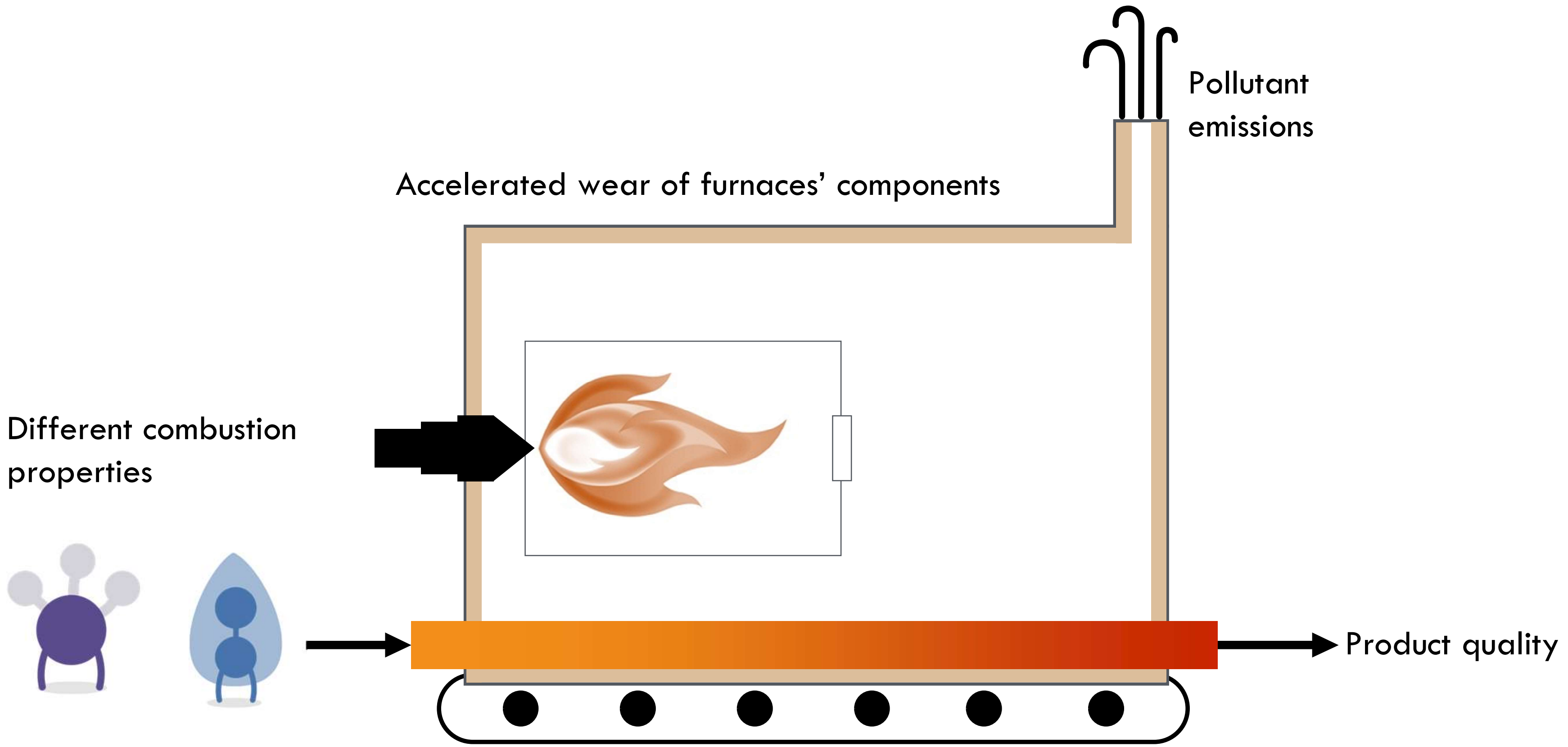
NOx reduction:

- 91%, from 633 ppm (A-type) to 57 ppm (C-type), φ_1=1.15
- 64%, from 1594 ppm (A-type) to 575 ppm (C-type), φ_1=1.45

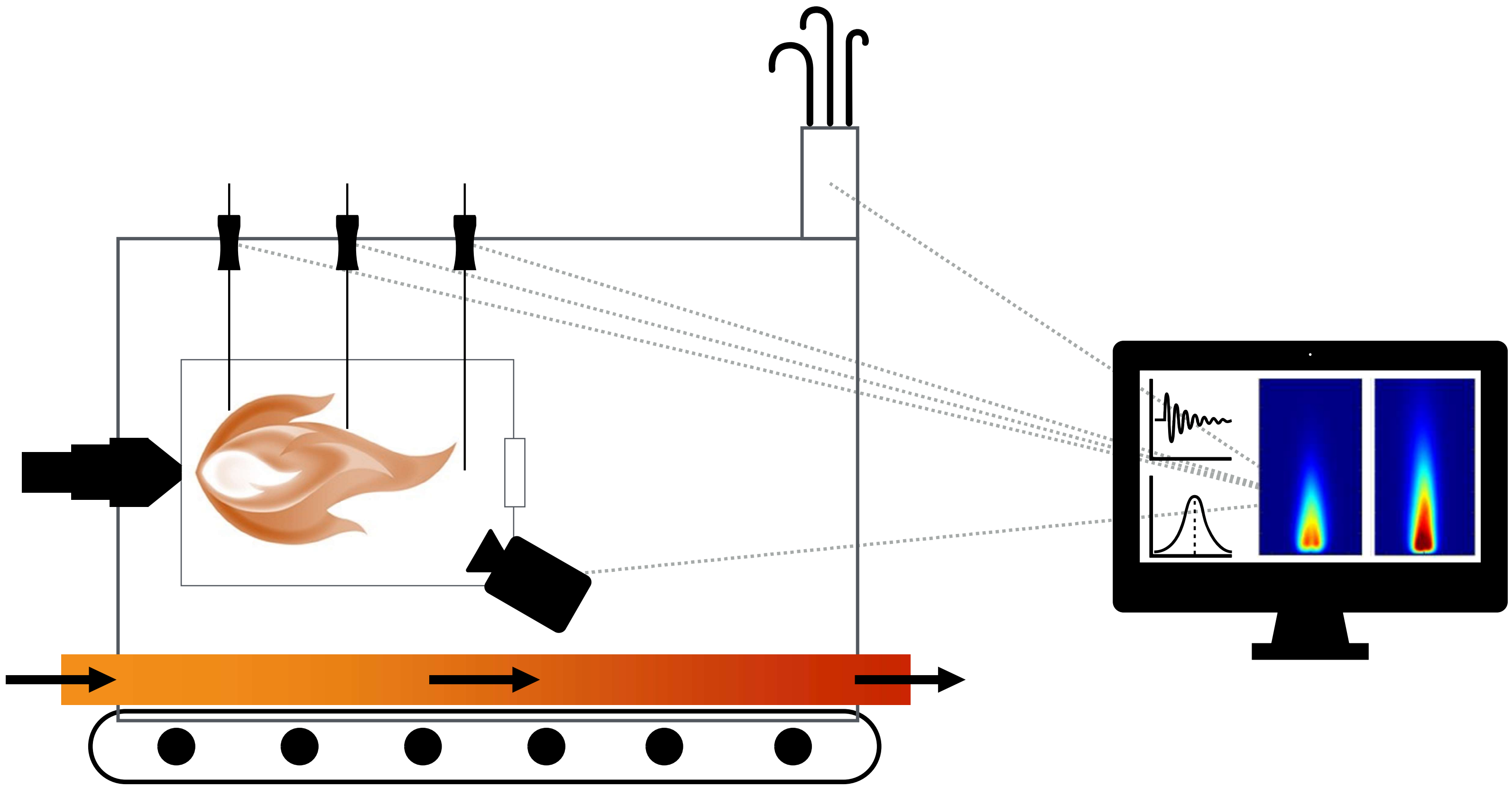
The design allows for an in situ SNCR limiting NO formation in the second stage



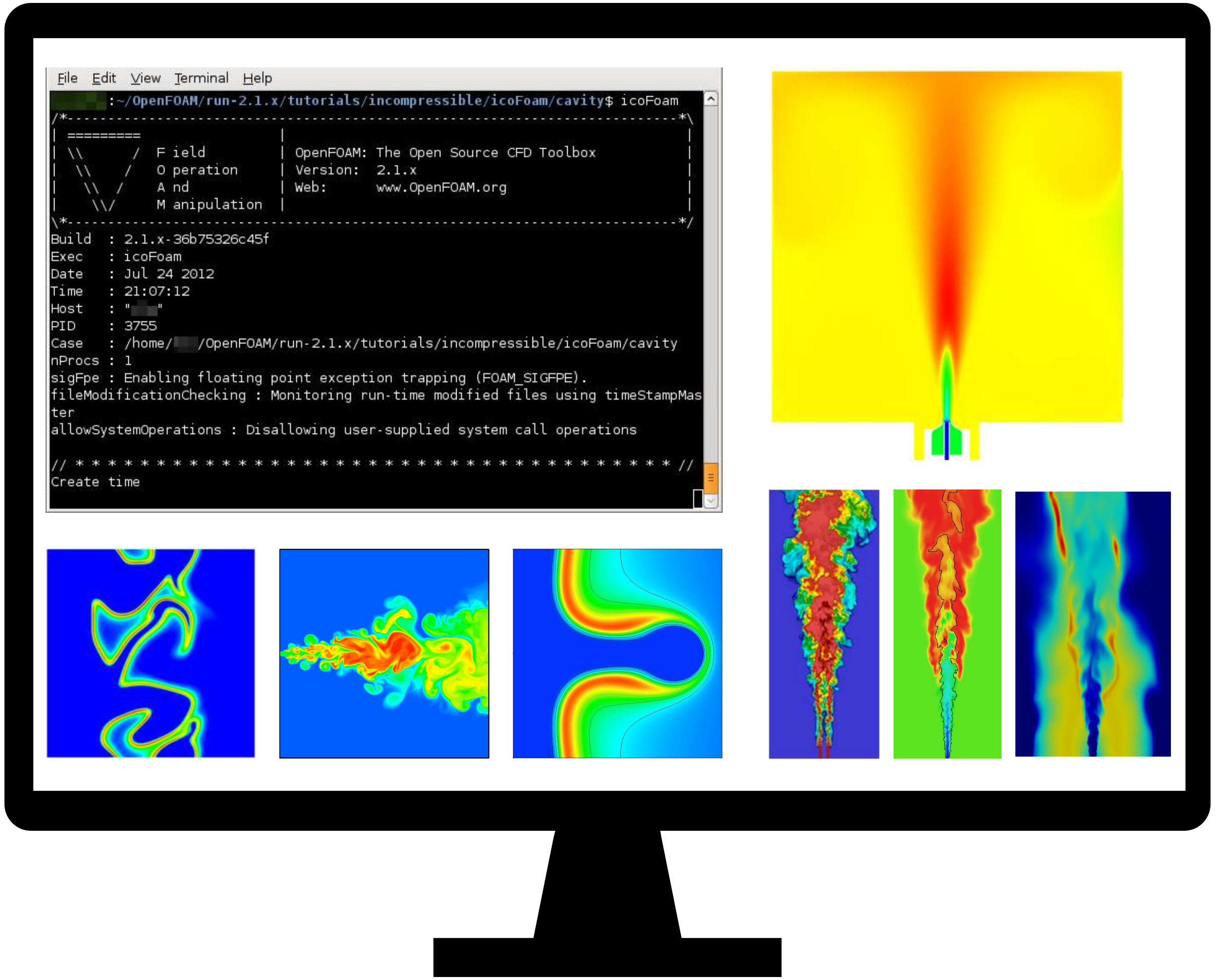
Relying on RSFs raises a number of questions and technological challenges that remain to be answered



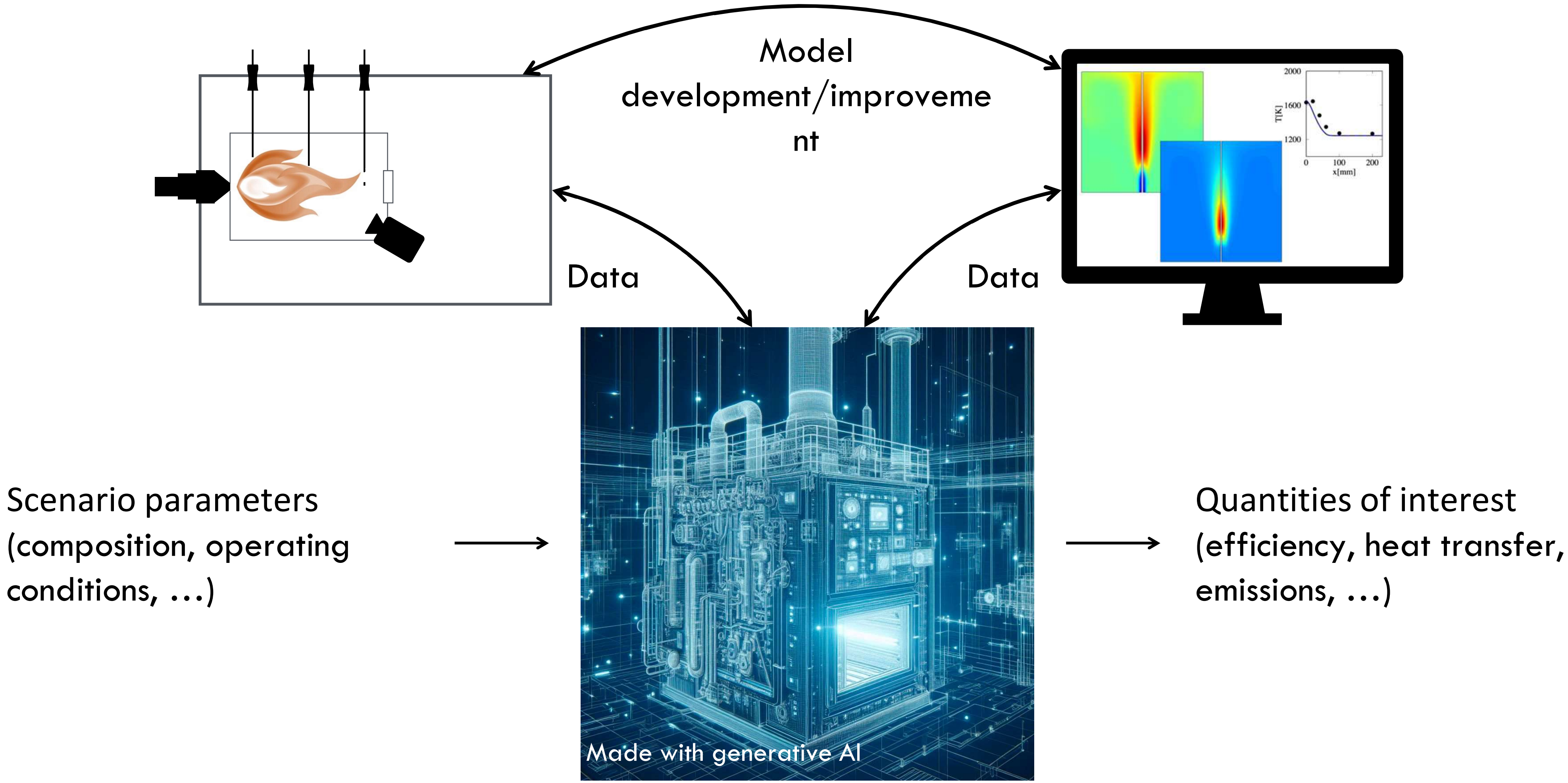
Diagnostics is helpful but limited in harsh combustion environments



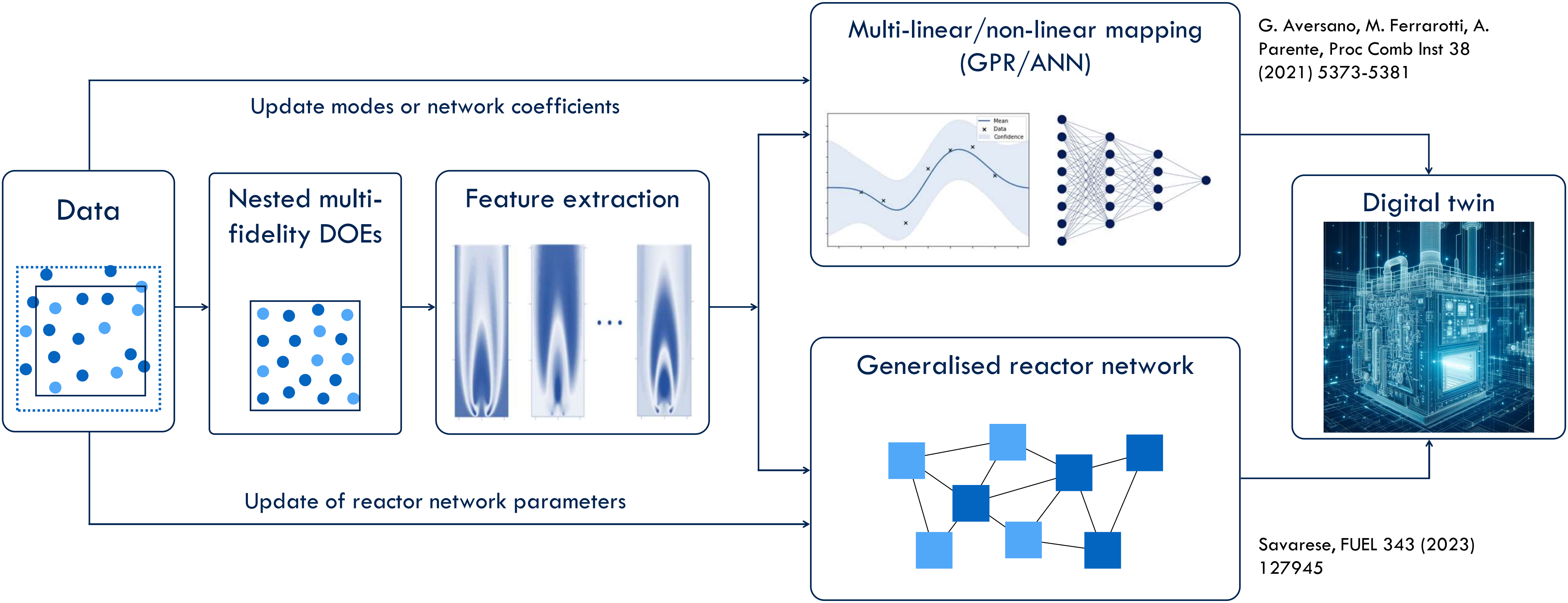
High-fidelity fidelity simulations are unsuitable for practical combustion systems



We shall combine theory, experiments and numerical simulations into digital twins to decarbonise industrial heat



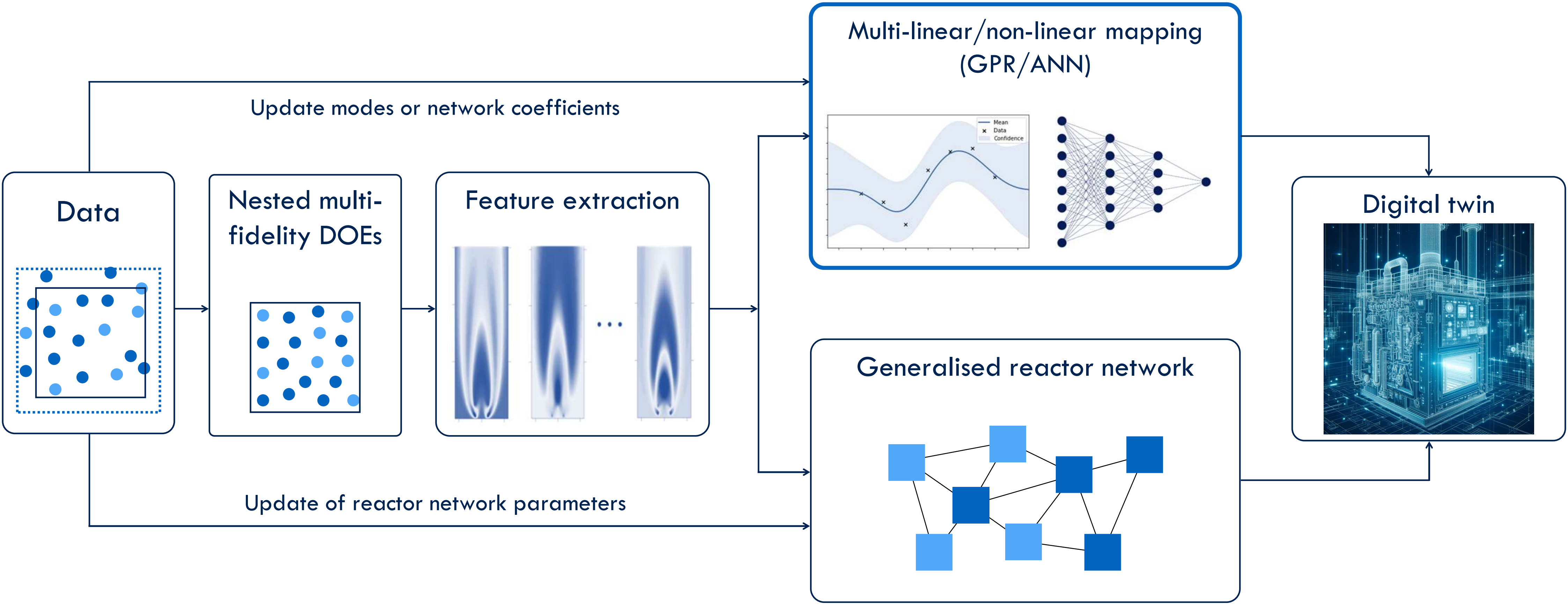
Strategies for DT development



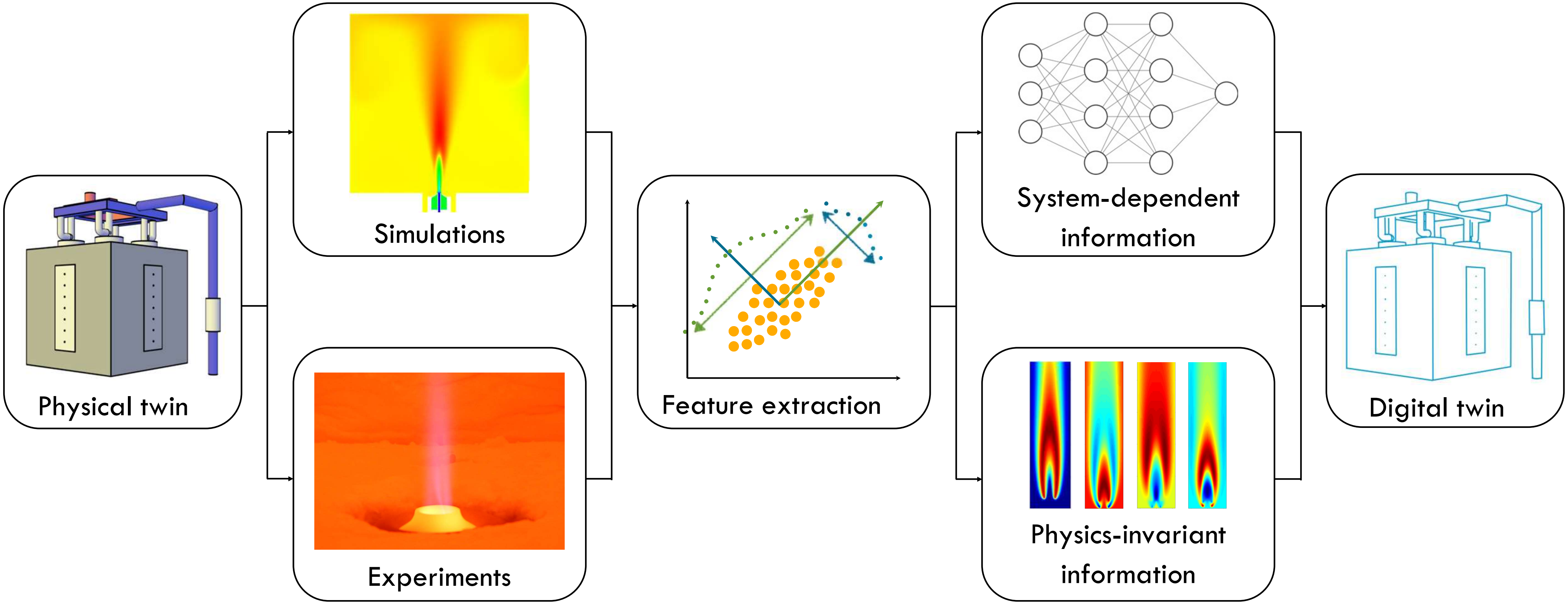
G. Aversano, M. Ferrarotti, A. Parente, Proc Comb Inst 38 (2021) 5373-5381

Savarese, FUEL 343 (2023) 127945

Strategies for DT development

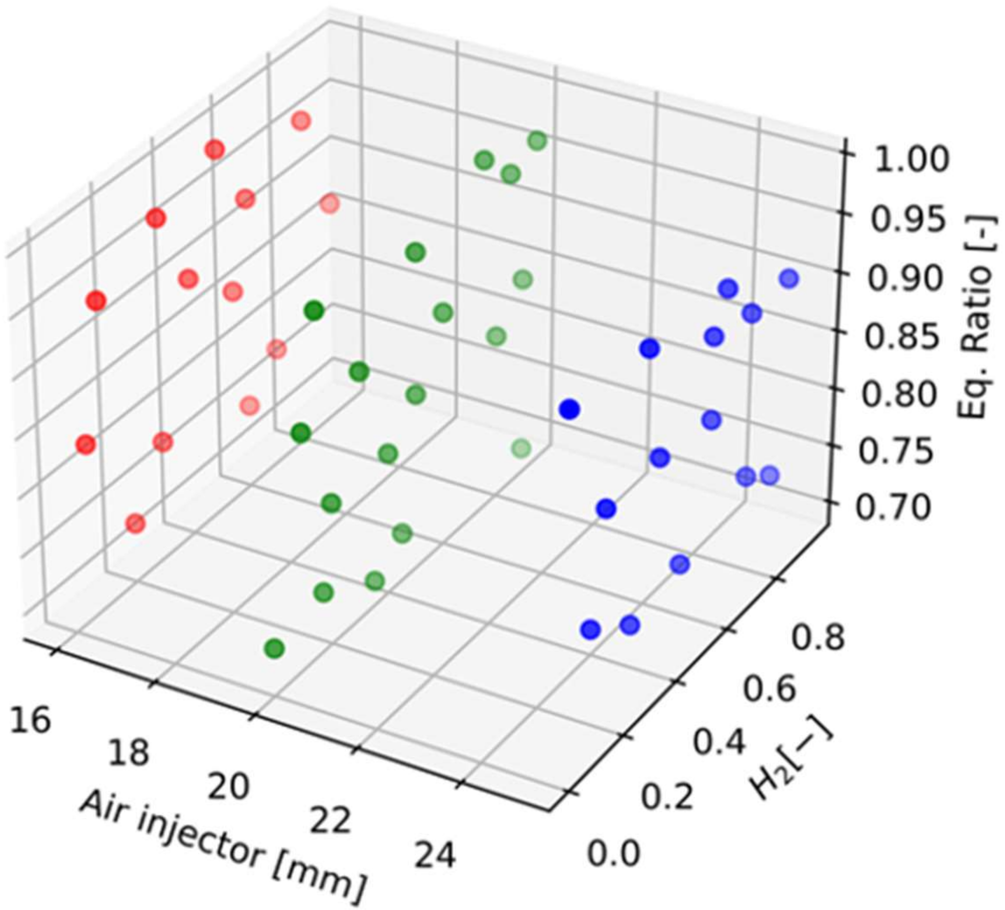


We have designed an approach to develop digital twins of complex combustion systems



G. Aversano, M. Ferrarotti, A. Parente, Proc Comb Inst 38 (2021) 5373-5381
Distinguished paper, Stationary Combustion Systems

We explored the furnace behaviour in a broad range of conditions (fuel/air charge, internal aerodynamics)

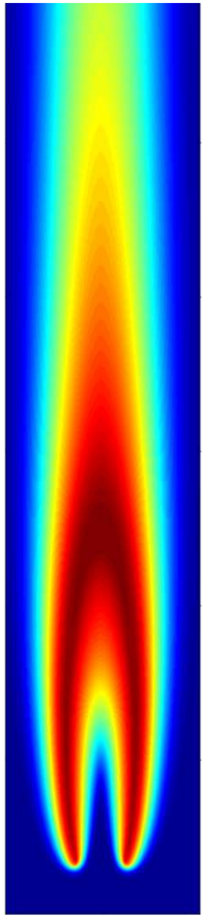


50+ CFD simulations (3D RANS)

3 input parameters

In our approach, any scalar field becomes the weighted sum of eigenflames through system-dependent coefficient

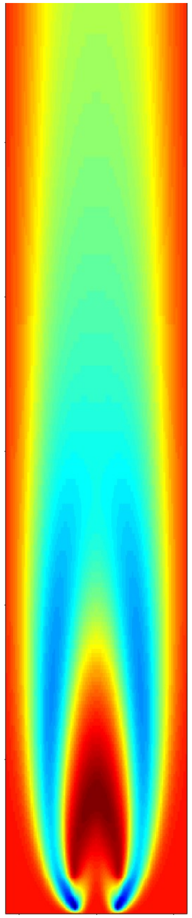
Temperature



$$= \mathbf{a}_1(\mathbf{x}) \cdot$$

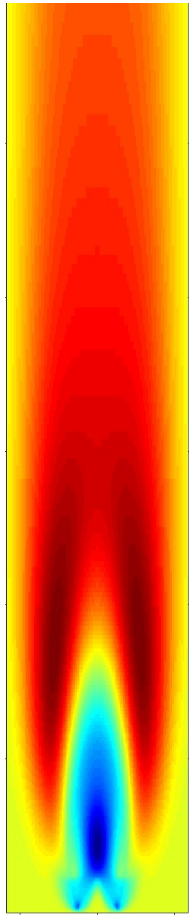
ML models

Eigenflame #1



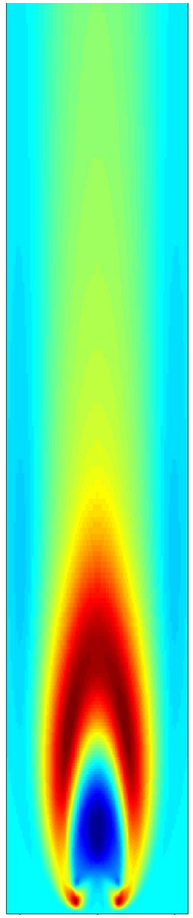
$$+\mathbf{a}_2(\mathbf{x}) \cdot$$

Eigenflame #2



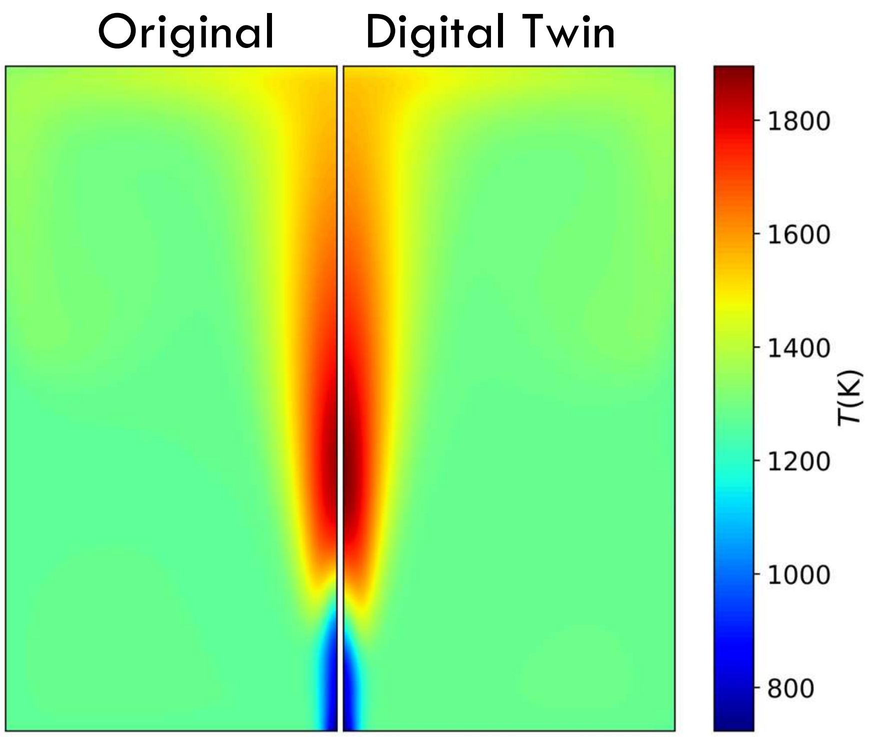
$$+\mathbf{a}_3(\mathbf{x}) \cdot$$

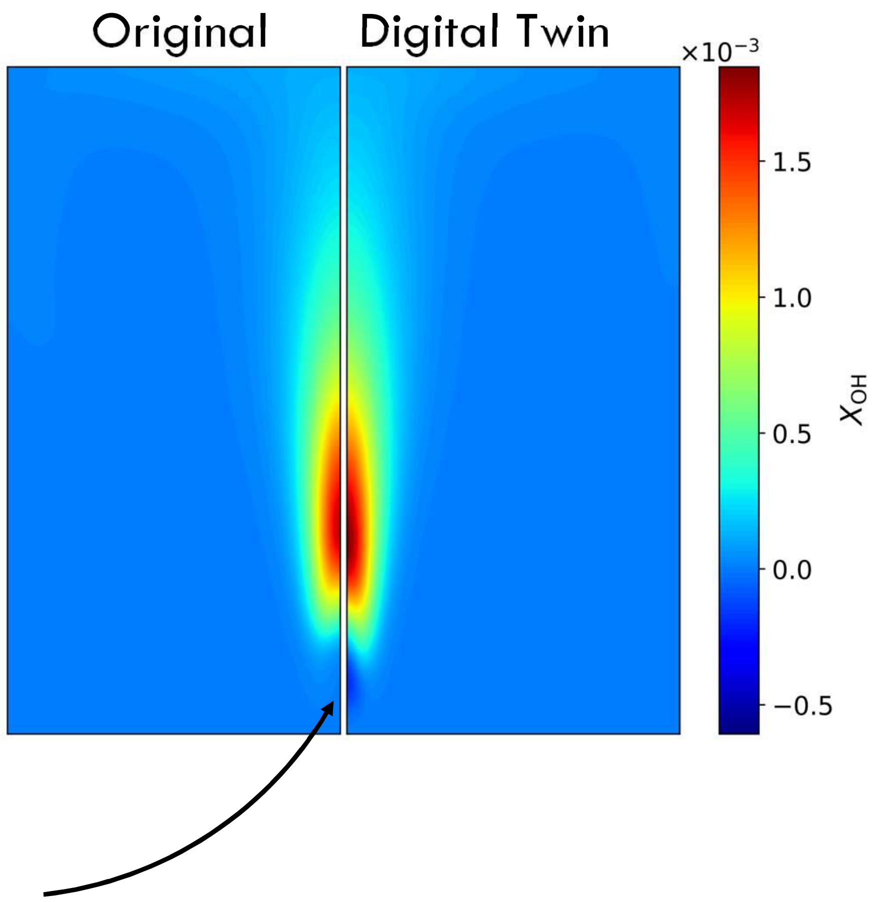
Eigenflame #3



$$+\ldots$$

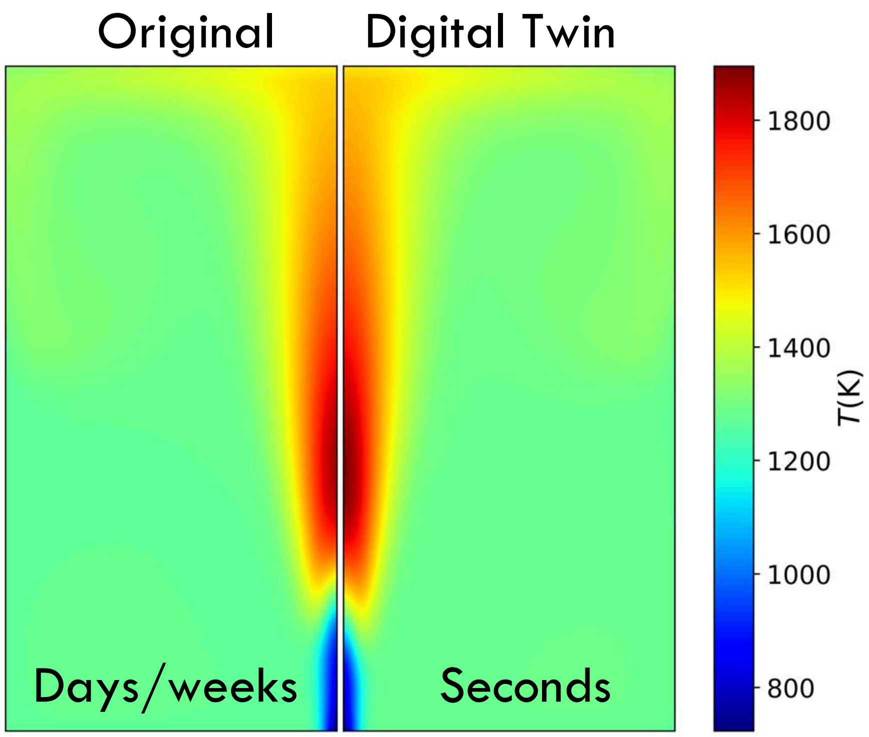
The DT reaches high level of accuracy

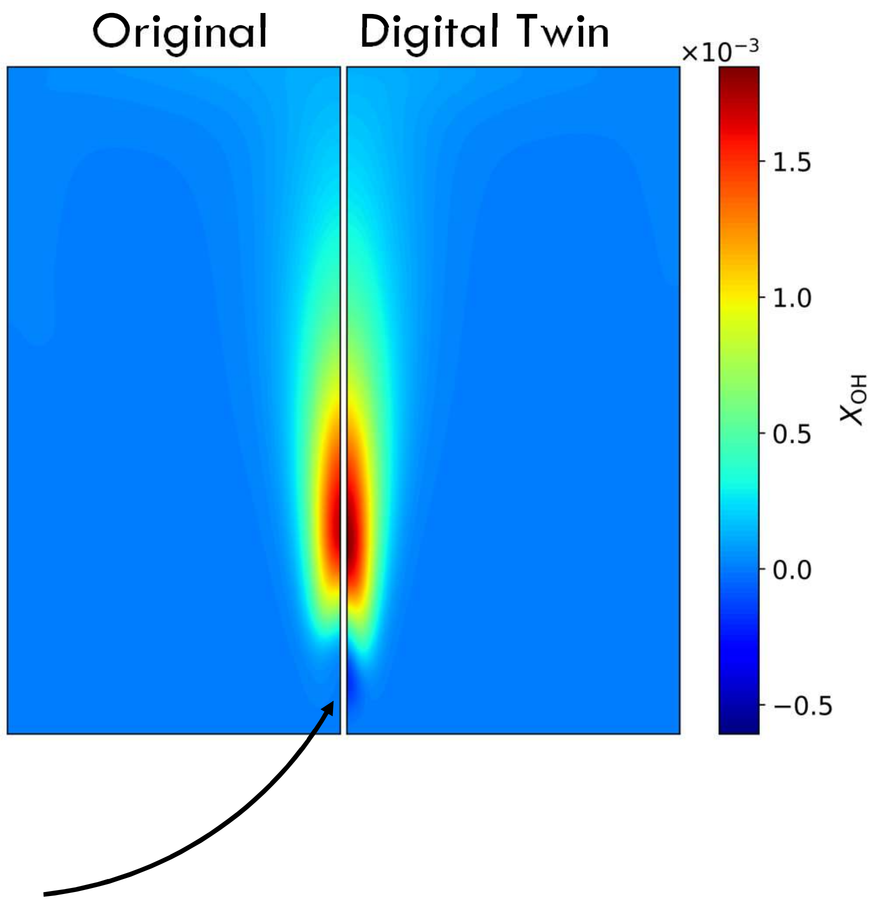




But there is still room for improvement

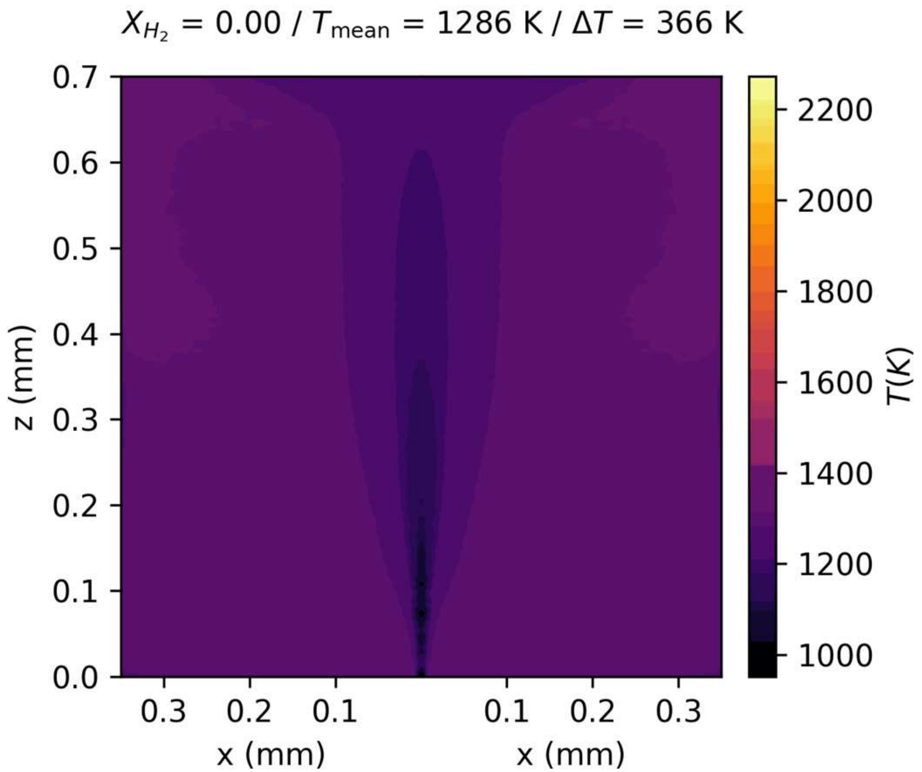
The DT reaches high level of accuracy

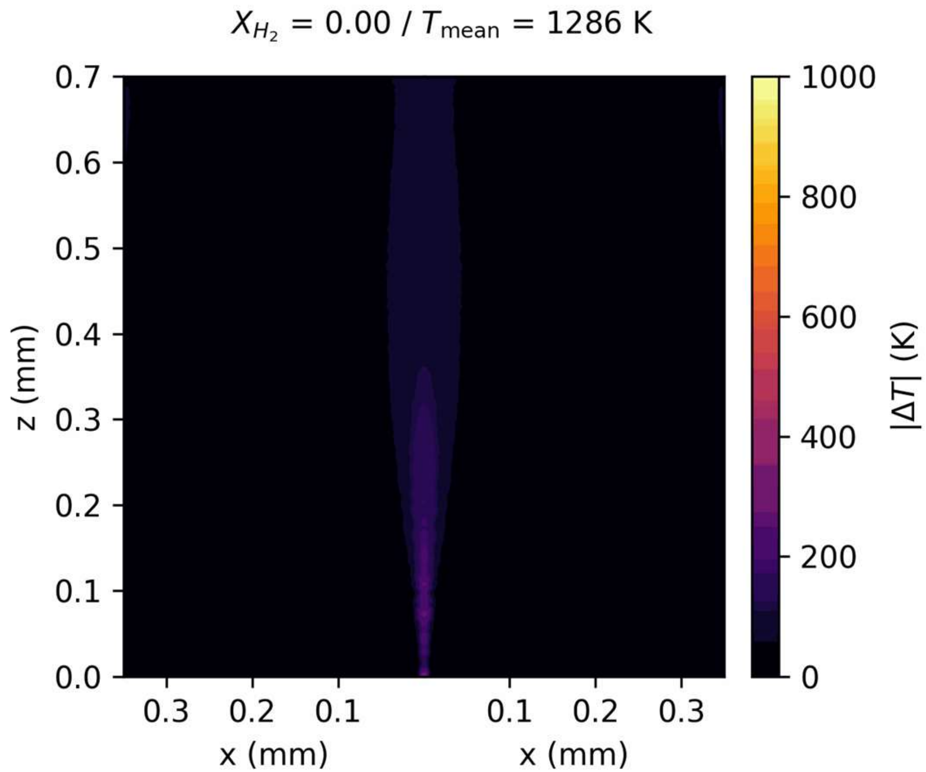




But there is still room for improvement

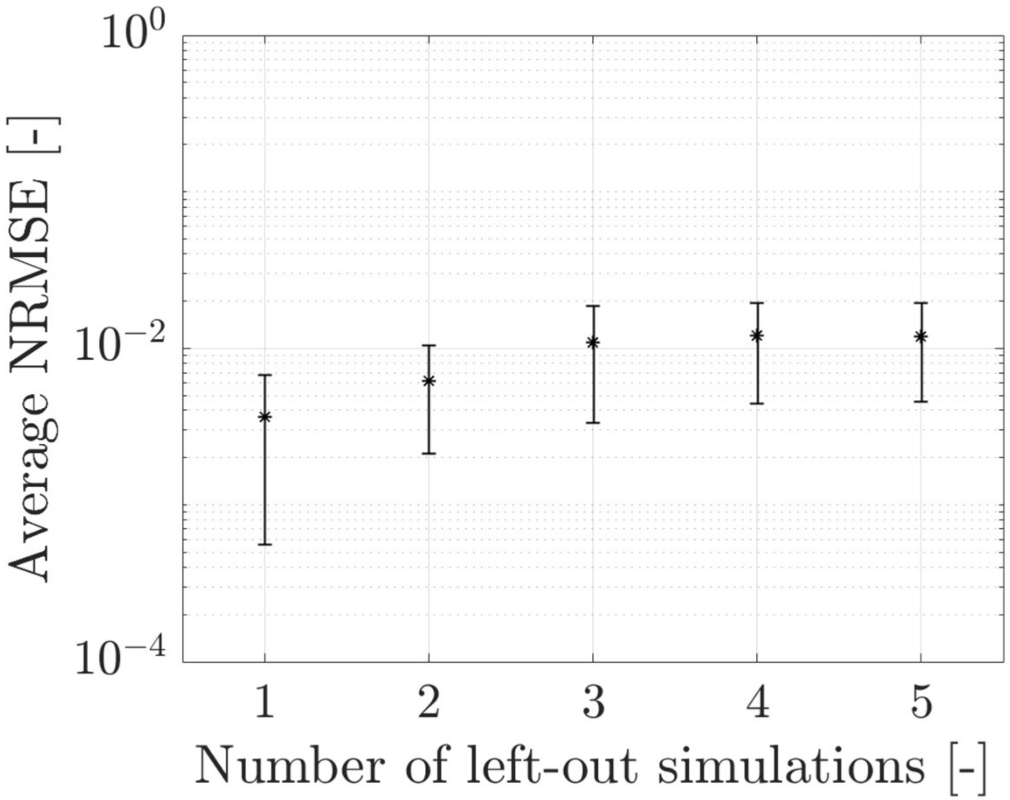
The GPR-based DT is capable of exploring a broad range of states in the DOE space



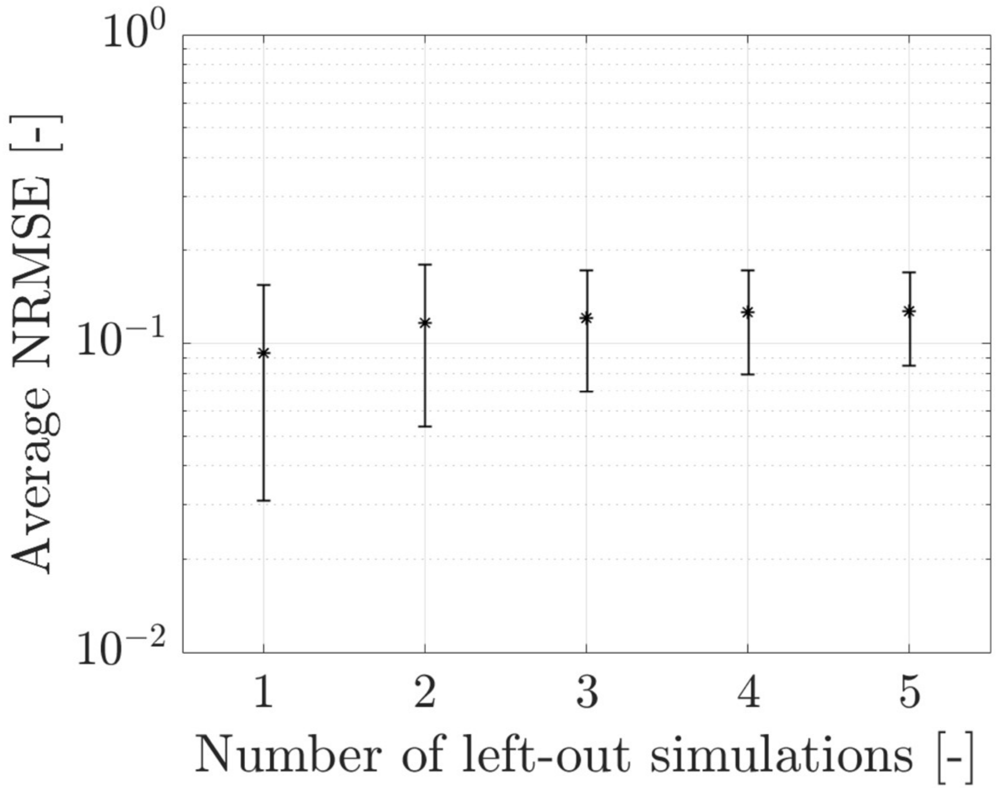


Leave-k-out reconstruction and prediction metrics

Reconstruction



Prediction

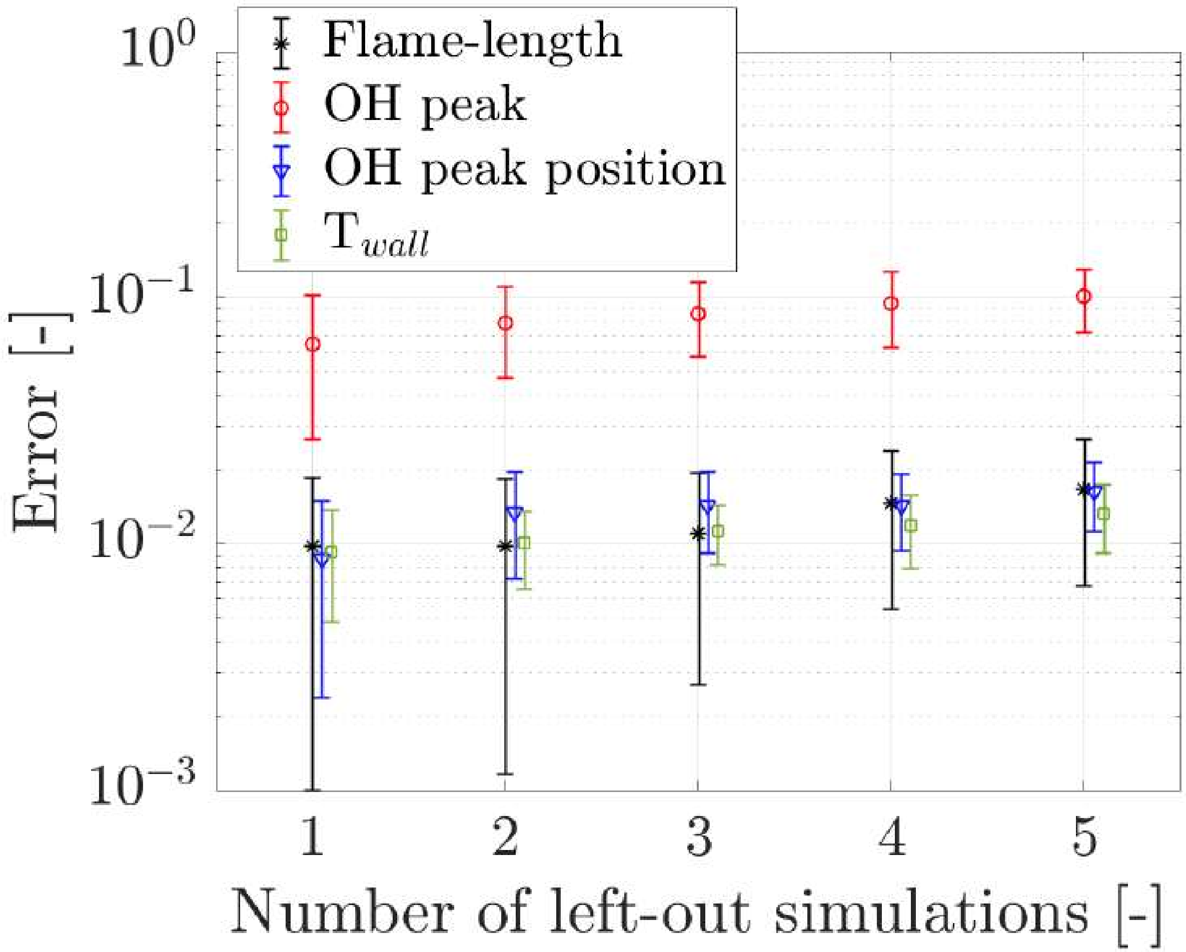


A reduced-order model for the quantities of interest

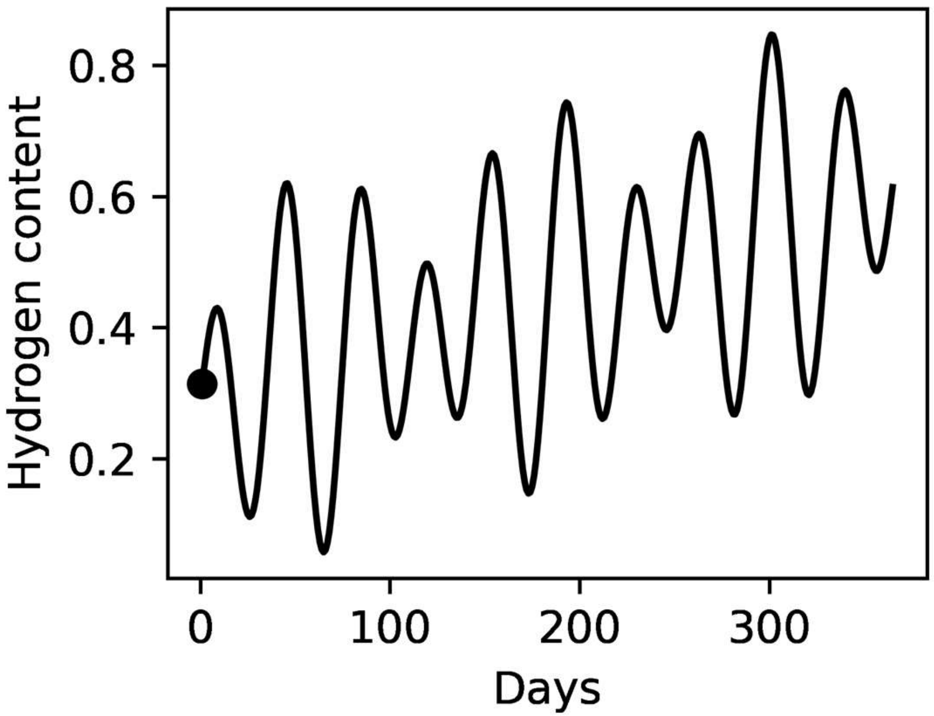
What are the true quantities of interest in a digital twin?

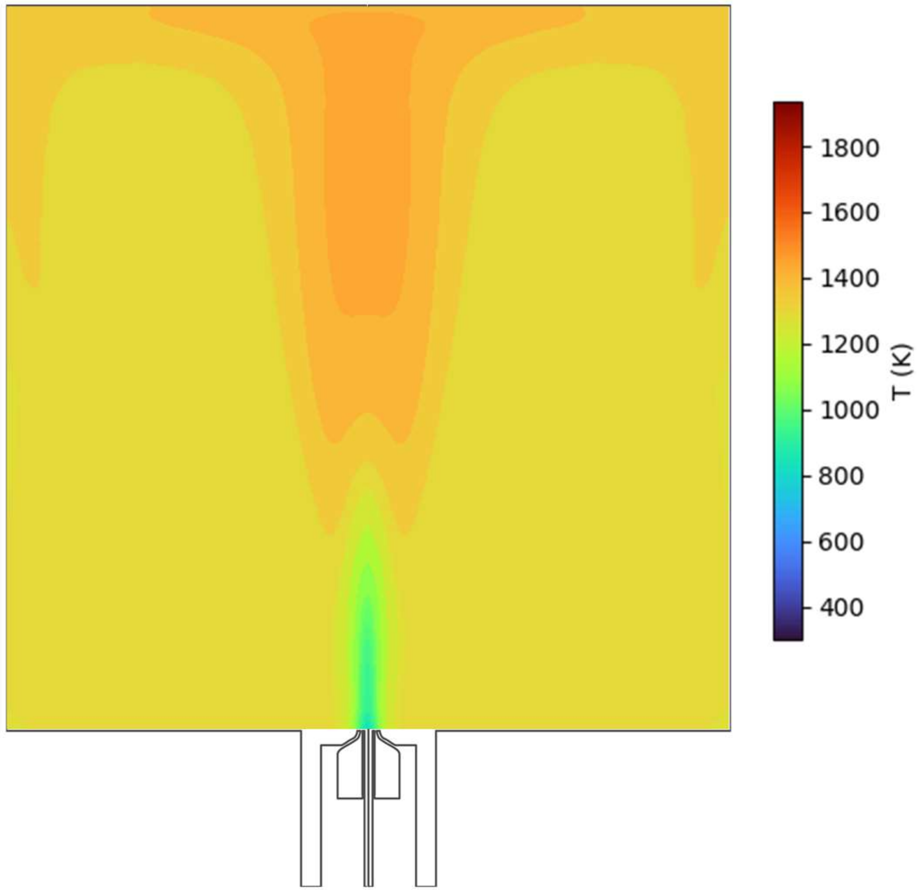
- Max temperature
- Wall temperatures
- Flue gas composition
- Flame length, OH peak value & location (soft sensing)

A reduced-order model for the quantities of interest



The DT allows us to explore the systems states for changes at the boundaries (e.g. load)



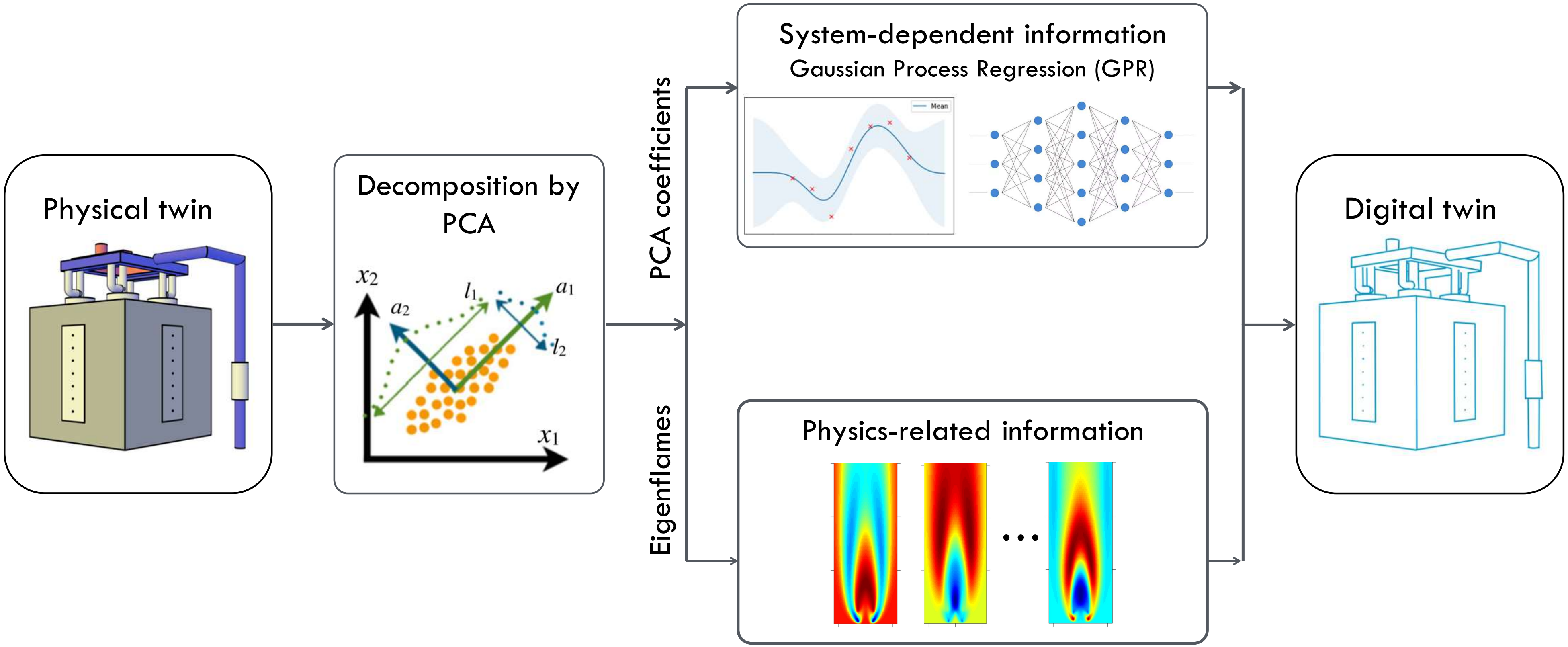


Once a DT is built, can we update/upgrade it?

Upgrade a simulation-based DT with few experimental data

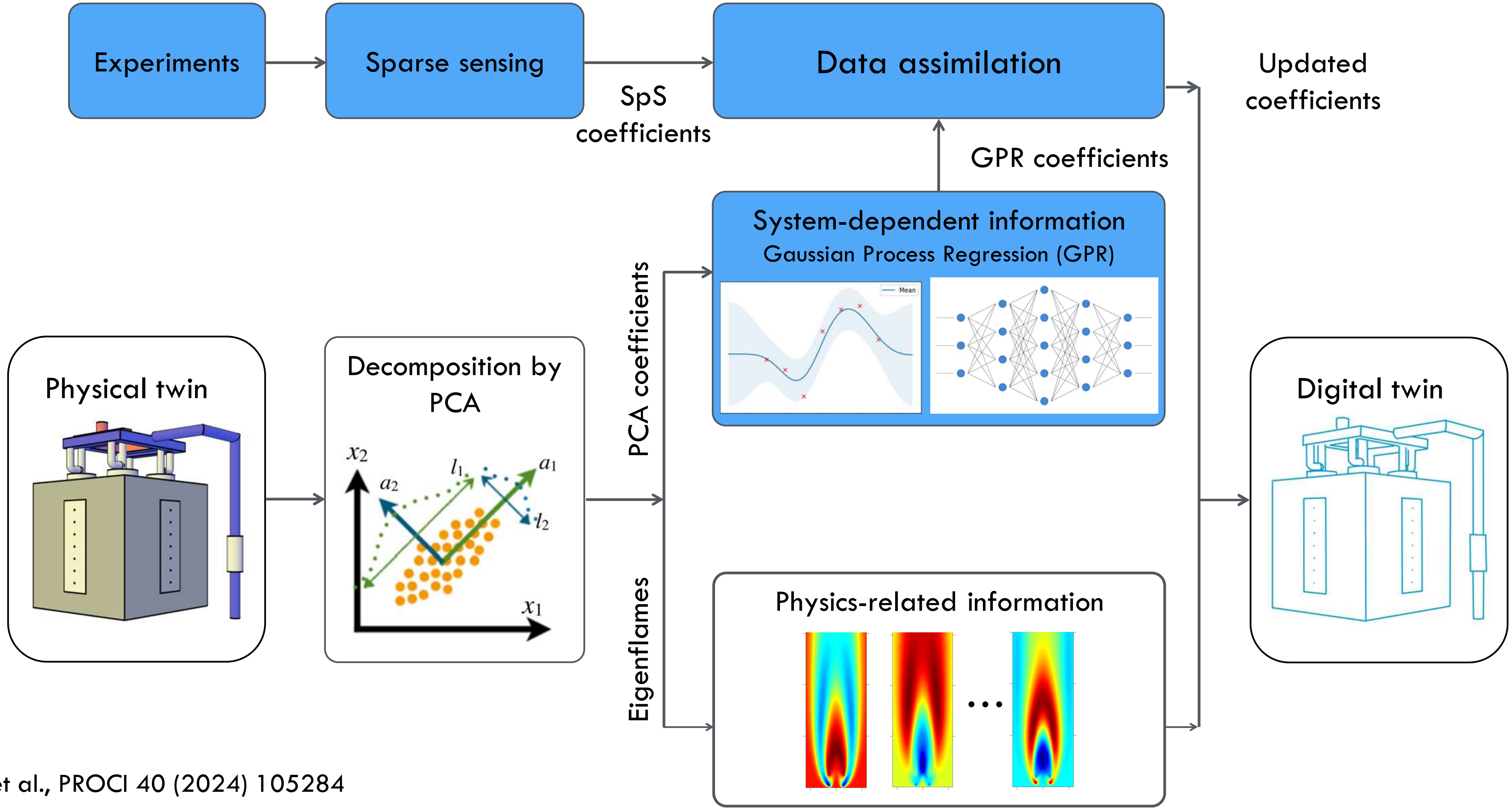
Update some components of the reduced-order model

Update the DT with experimental data



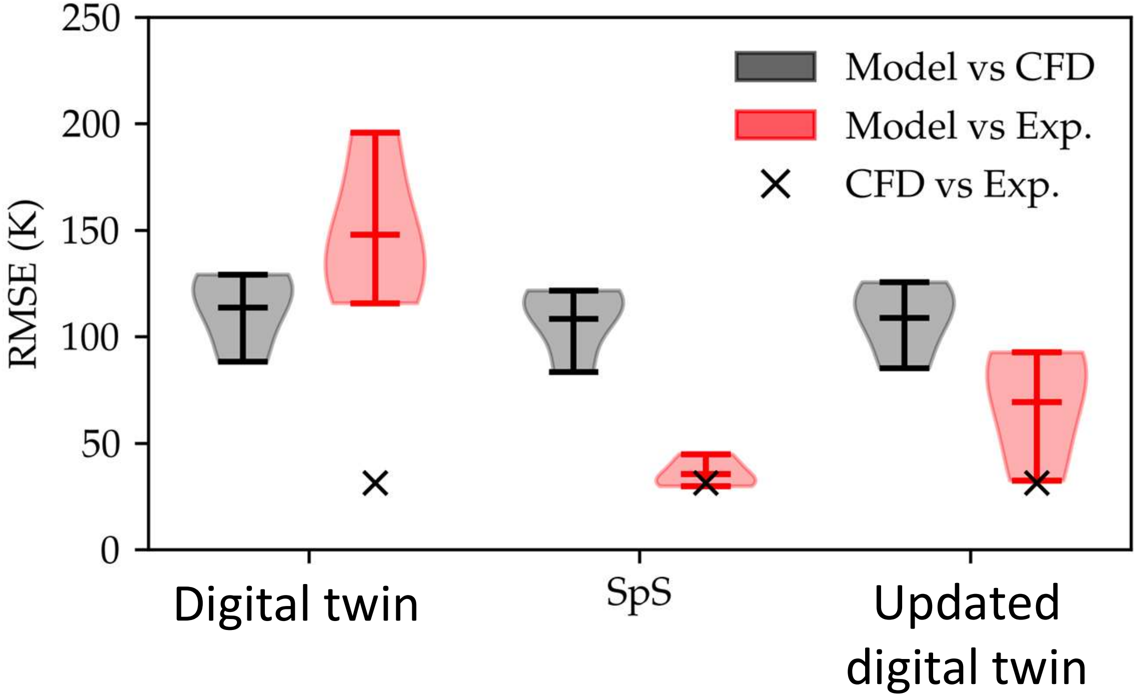
G. Aversano, M. Ferrarotti, A. Parente, Proc Comb Inst 38 (2021) 5373-5381
Distinguished paper, Stationary Combustion Systems

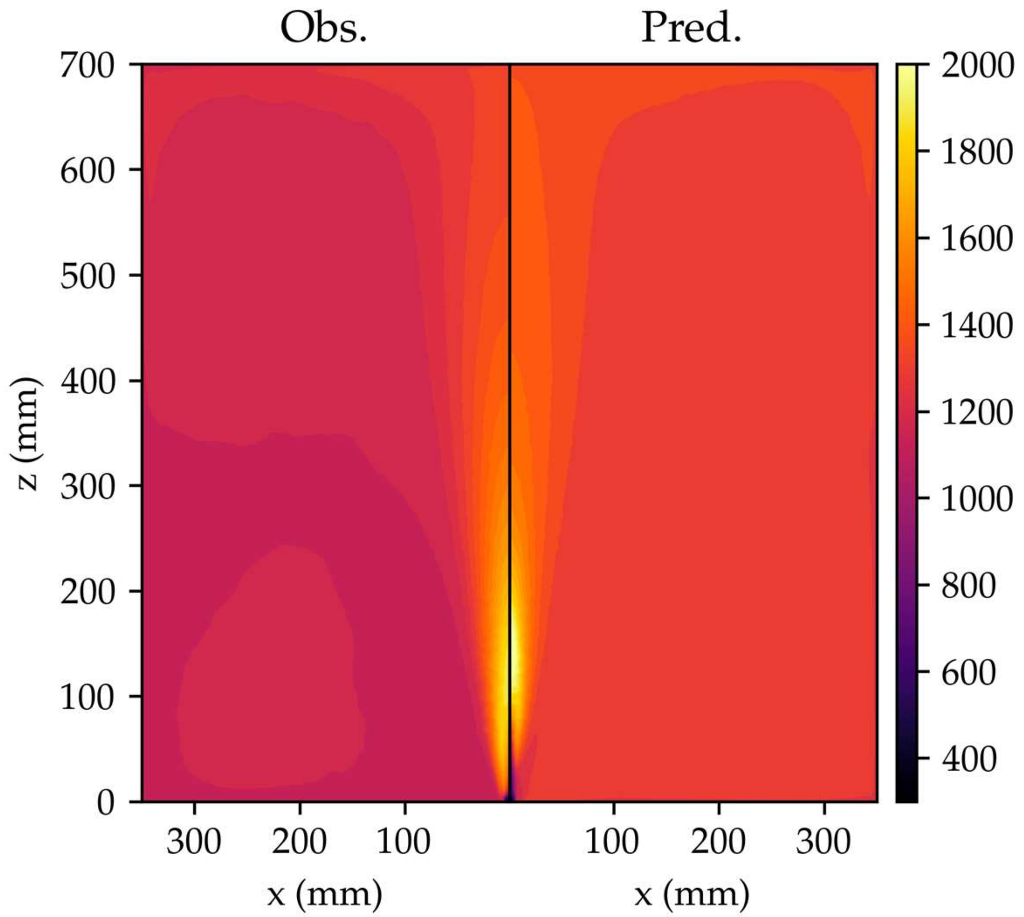
Update the DT with experimental data



Donato et al., PROCI 40 (2024) 105284

The update process continuously improves the ROM based on data from sensors





Donato et al., PROCI 40 (2024) 105284

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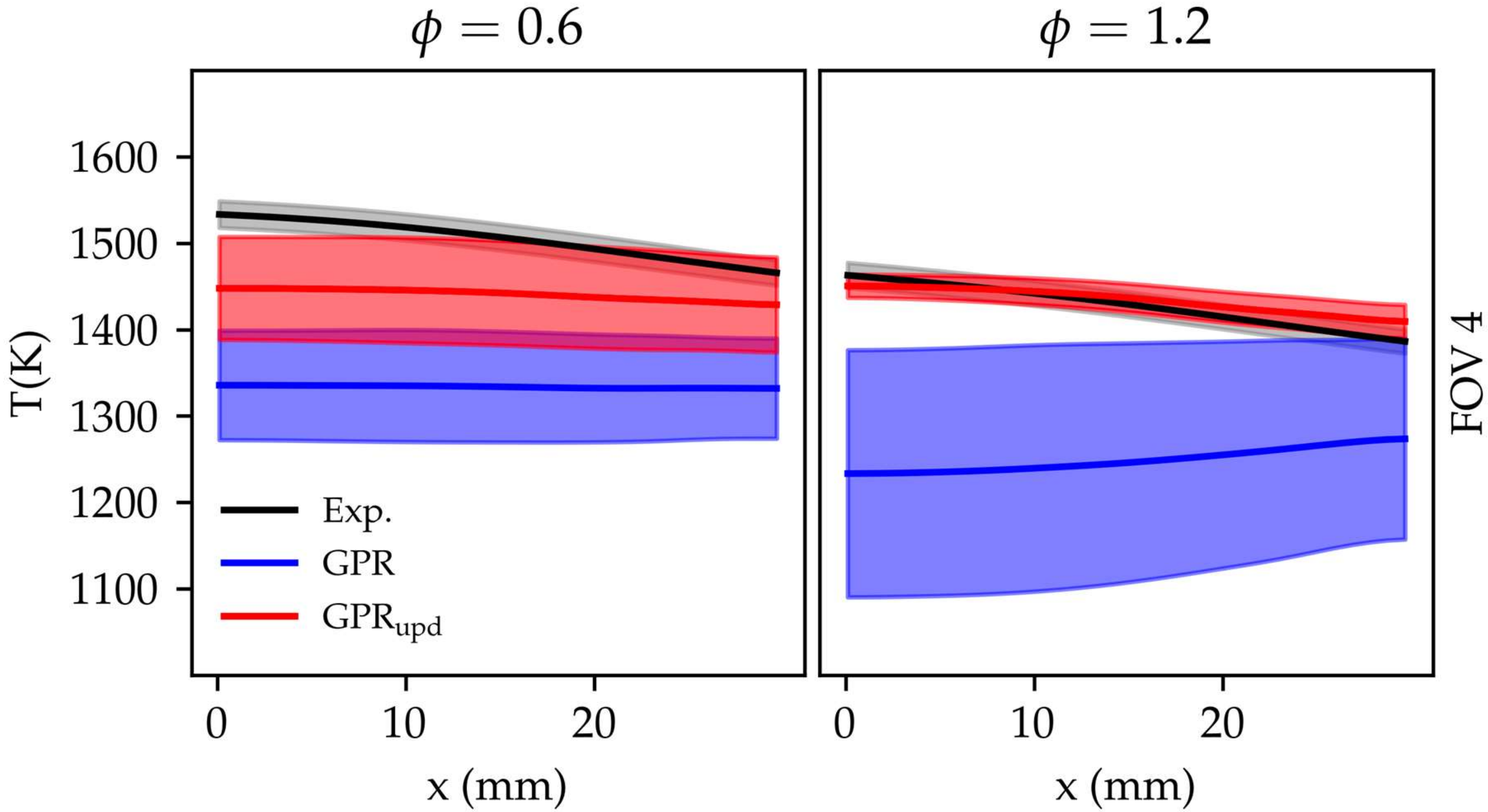

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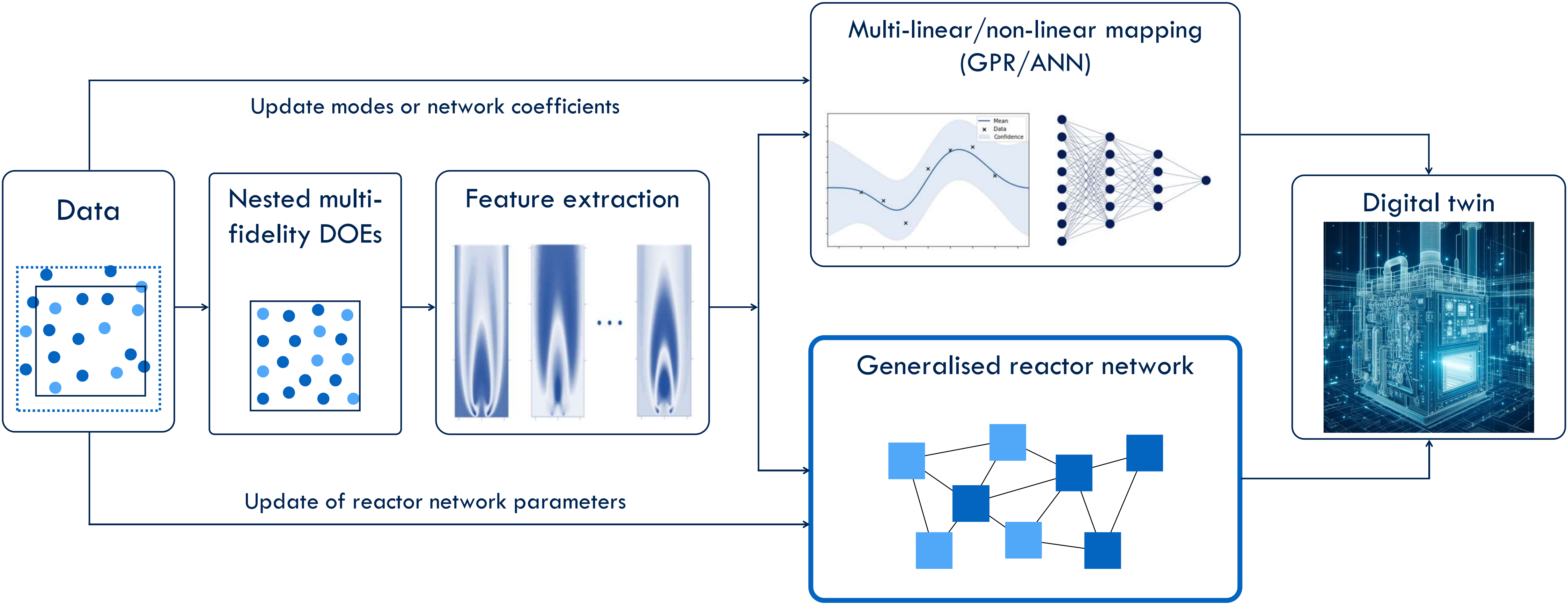
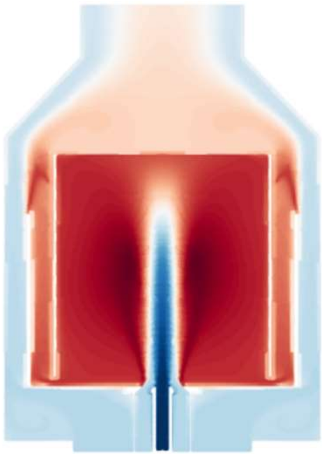
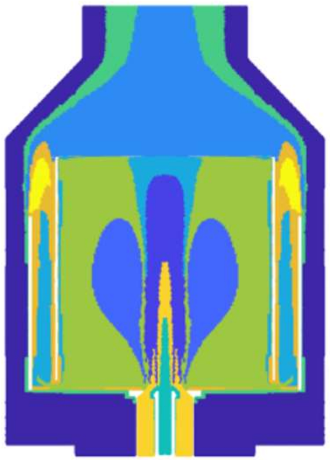
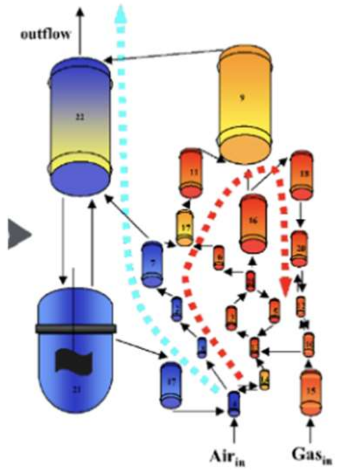
Strategies for DT development



The advantage of CRN-based DT is that physics is preserved by construction

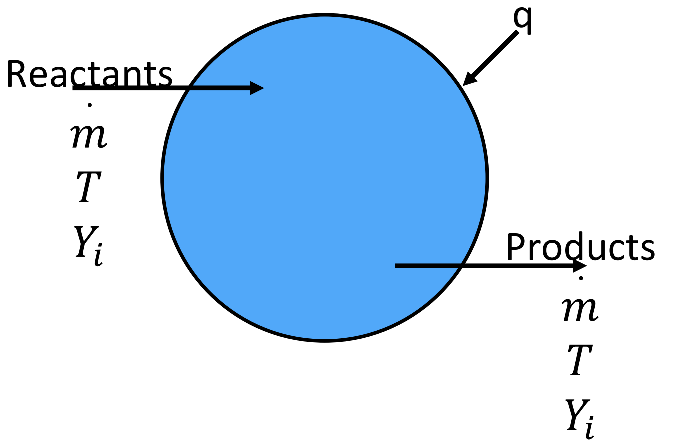






Physics-based simulation	Unsupervised Learning	CRN simulations
High detail Manageable kinetics High computational cost	Identification of key zones with similar thermo-chemical properties	Lower detail (but physics-based) Detailed kinetics Low computational cost

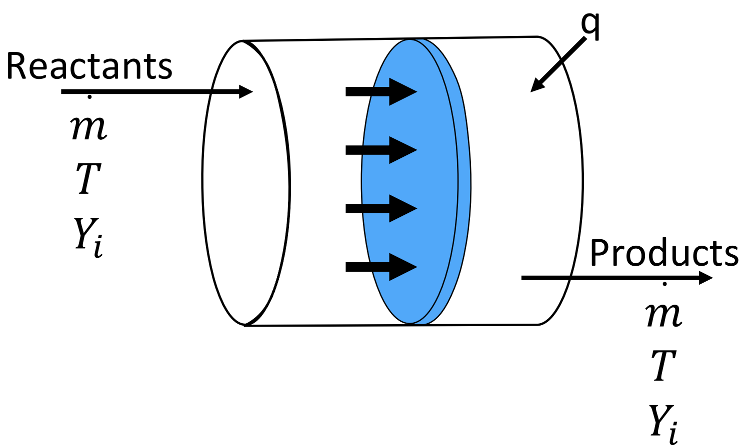
The system behaviour is described using a combination of 0D or 1D chemical reactors



Perfectly Stirred Reactor PSR

- Zero-dimensional
- Perfect mixing
- Constant volume
- Steady-state

$$\frac{dY_i}{dt} = \frac{Y_i^{inlet} - Y_i}{\tau} + \frac{\dot{\omega}_i}{\rho}$$

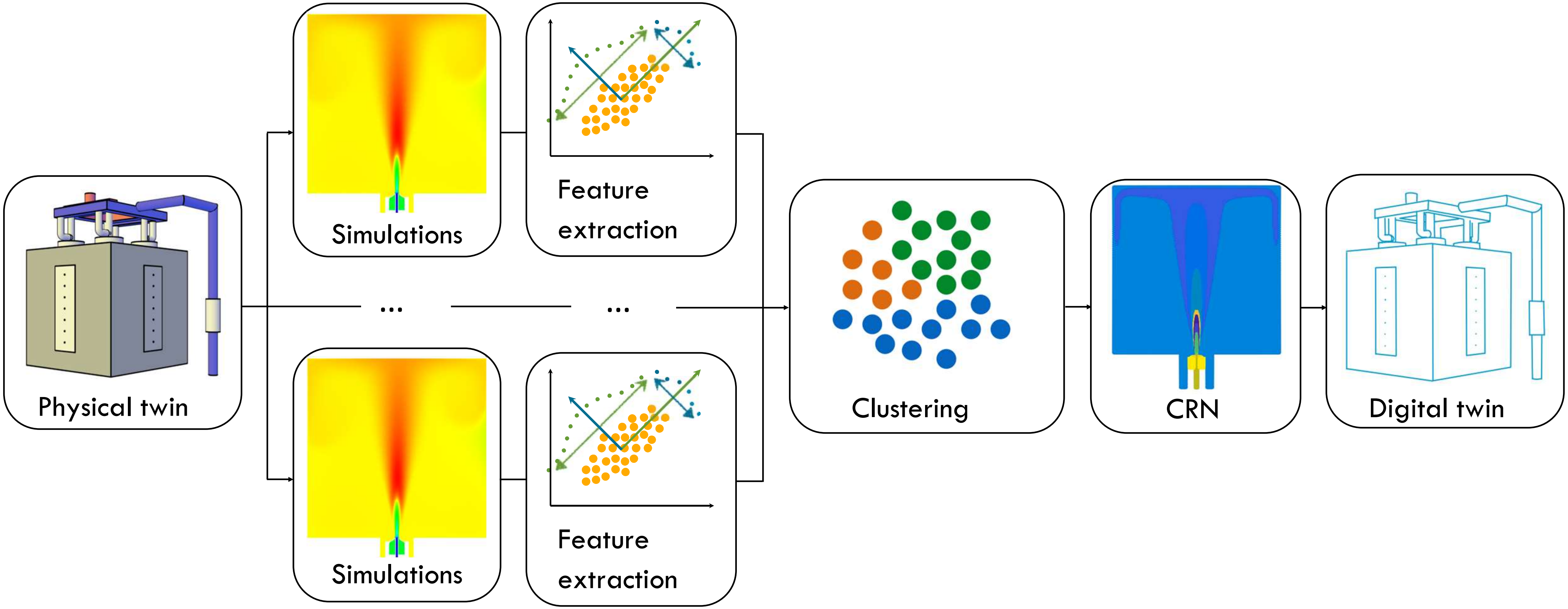


Plug Flow Reactor PFR

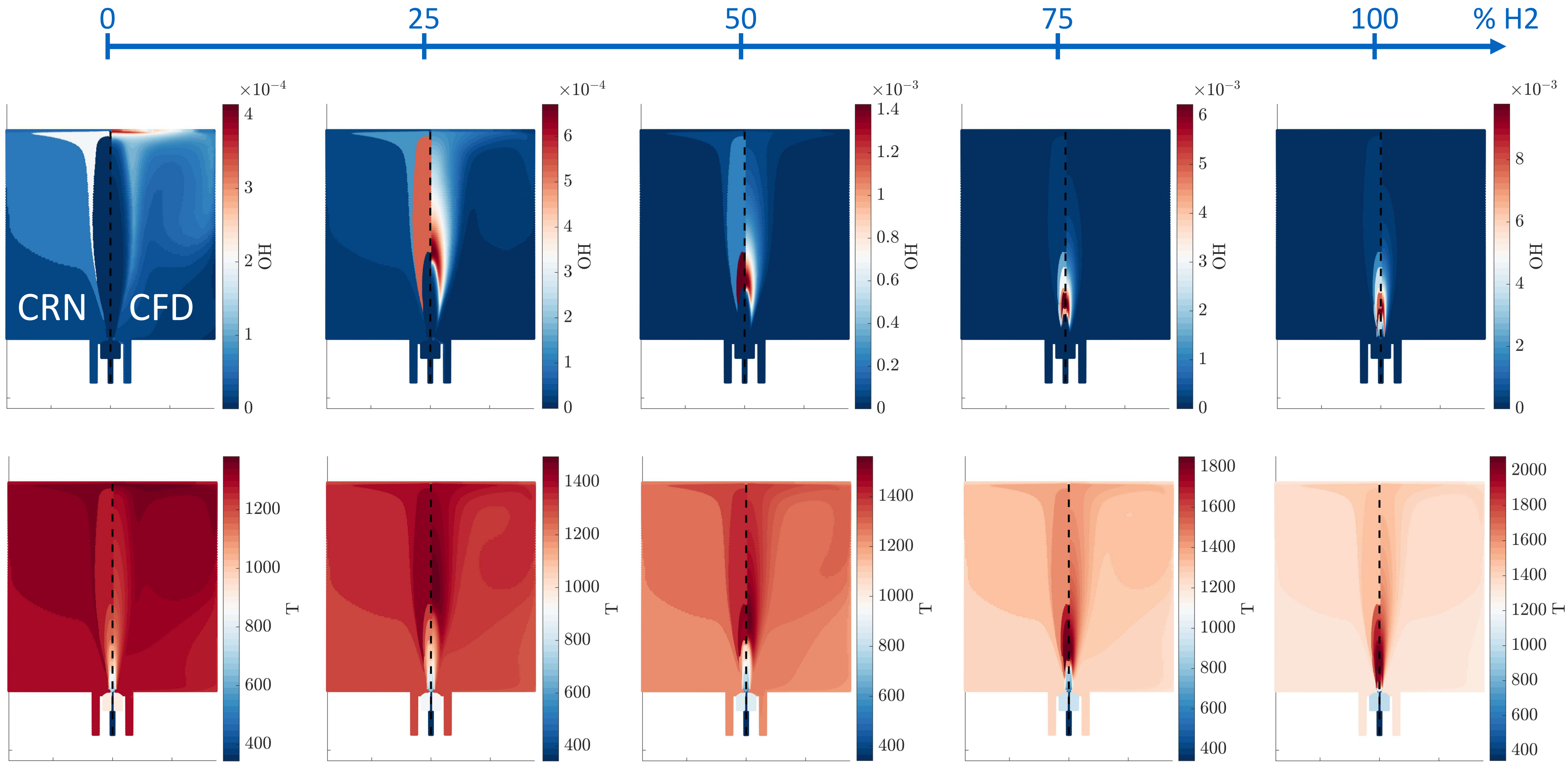
- One-dimensional
- No mixing or back flow
- Concentration gradient
- Steady-state

$$\frac{dY_i}{dt} = \frac{\dot{\omega}_i}{\rho}$$

The reactor network is obtained by clustering the latent features from multiple simulations



A single CRN is obtained, for a wide range of of conditions



Concluding remarks

In flameless/MILD, what matters is the overall process (fuel+burner+furnace)

O_2-enrichment enhances ammonia reactivity and allows stable MILD ammonia combustion, with reduced (but still high) NO_x emissions

Low-emission ammonia combustion is possible with staged or continuously-staged configurations

Low-emission ammonia combustion is possible with staged or (better) continuously-staged configurations

Acknowledgements

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