CFD modelling of flameless combustion: from natural gas to hydrogen

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tenova

ESTEP
European Steel Technology Platform
20 years together

H_2 FOR GREEN STEEL
3rd INTERNATIONAL CONFERENCE

meets

A CIRCULAR ECONOMY DRIVEN BY THE EUROPEAN STEEL

voestalpine
ONE STEP AHEAD.

PRIMETALS
TECHNOLOGIES

Techint Group

OUR FAMILY

USD **38.4** billion
Annual Revenues

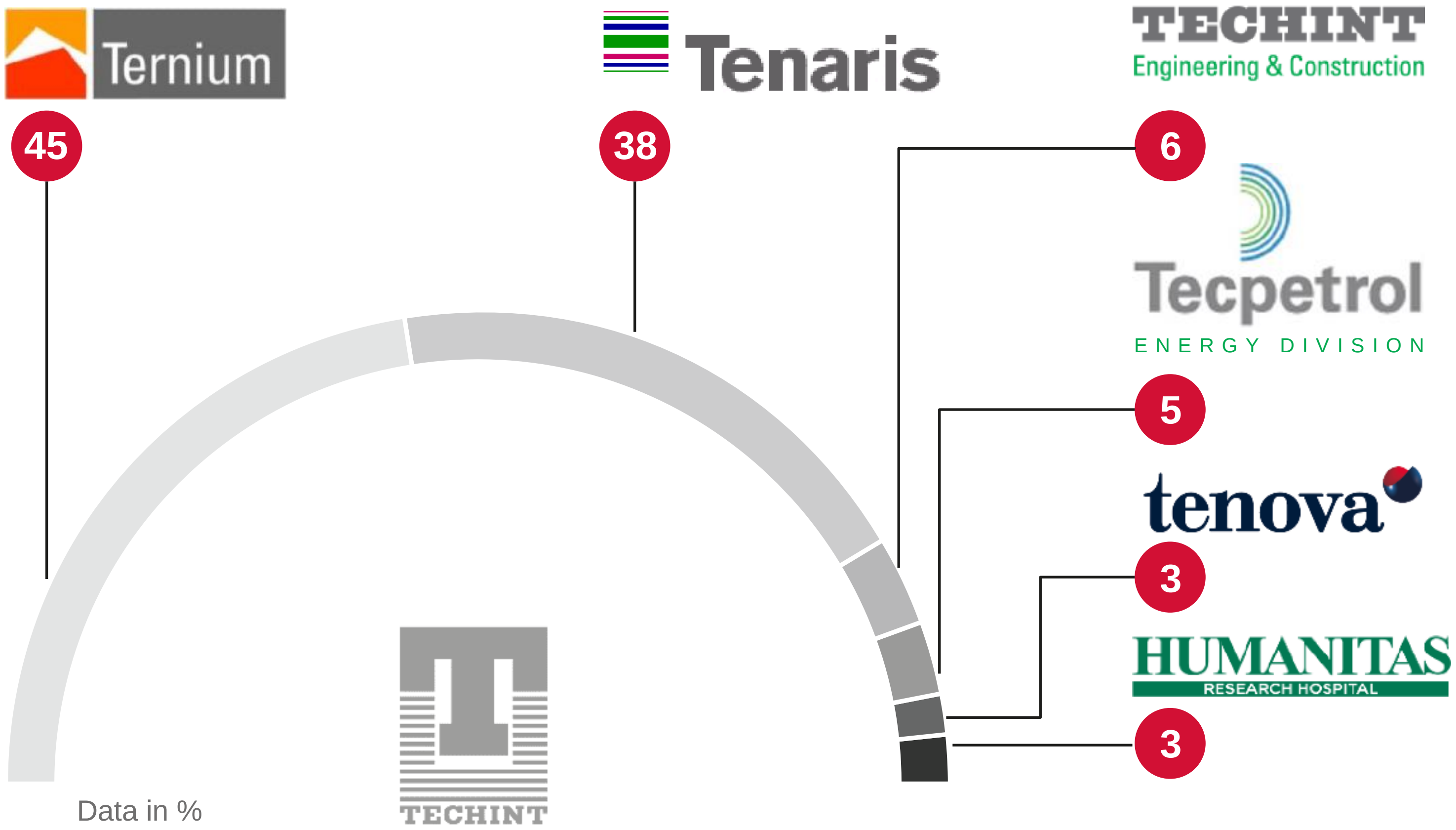
78,500
Permanent Employees

97,000
Total Employees

5
Continents

Revenues as of December 31, 2023

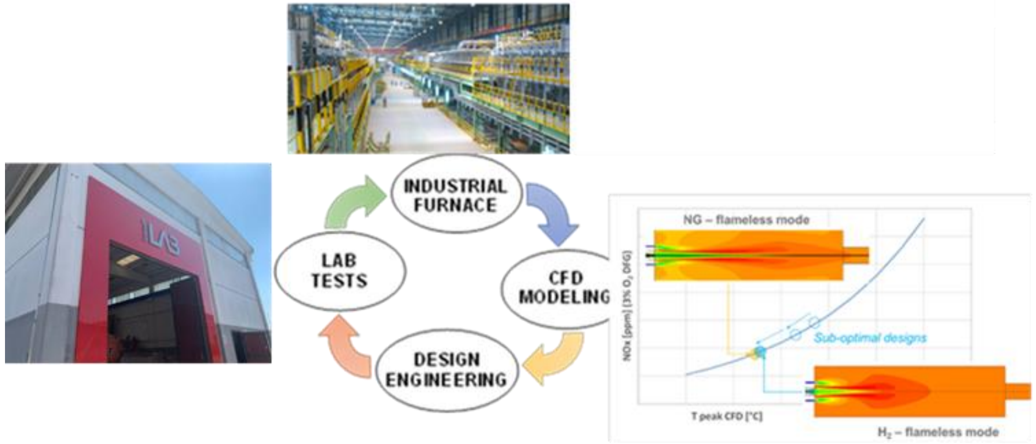
Six main Companies with operations worldwide



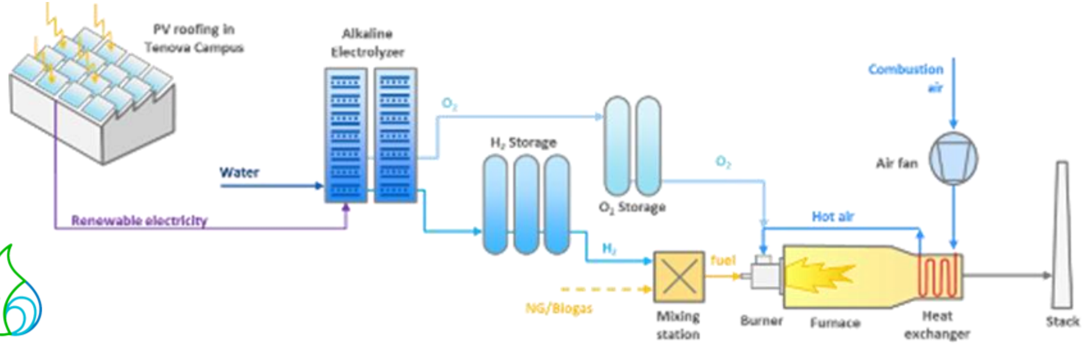
The problem

NEW TOOLS FOR NEW CHALLENGES

- Green H_2 combustion: very promising solution for downstream decarbonization
  - ✓ Potentially, 100% CO_2 reduction (Carbon Direct Avoidance)
- Tenova actively supports this transition: integrated development workflow with lab testing + modeling
  - ✓ R&D equipment upgrade, both lab testing and modeling



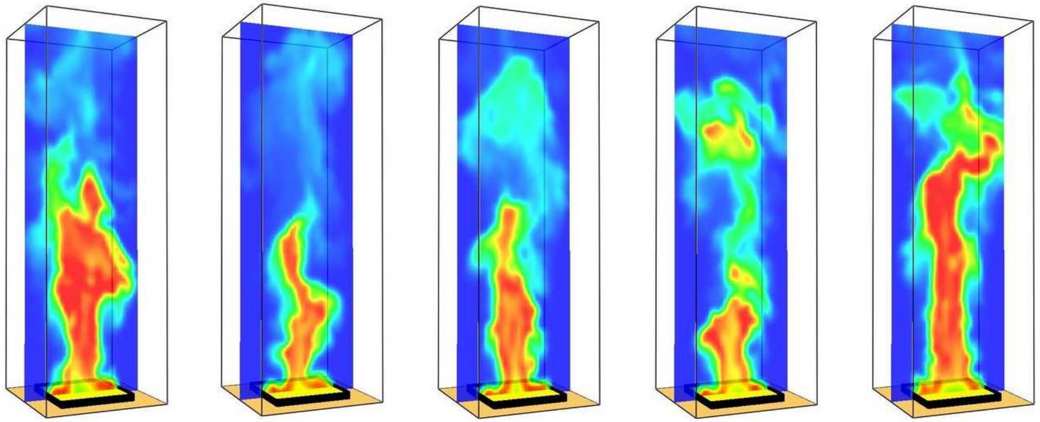
Experimental



HyTecHeat

- ✓ H_2 production
- ✓ Storage
- ✓ Distribution
- ✓ Mixing
- ✓ Control
- ✓ Safety

Modeling



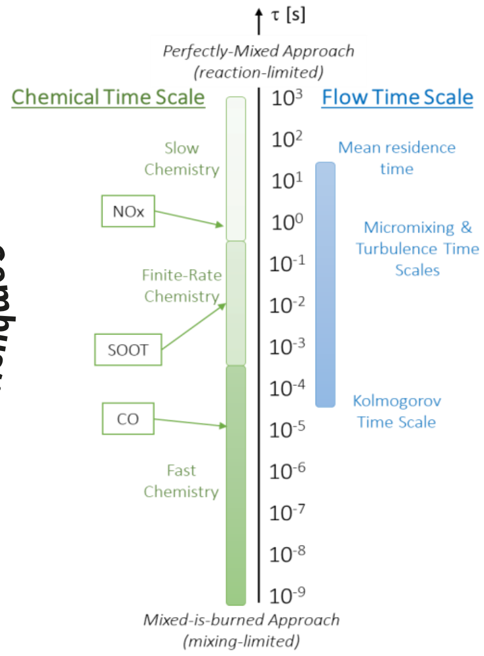
- ✓ Kinetic Mechanism
- ✓ NOx estimation
- ✓ Combustion model
- ✓ Radiation model

Combustion model

Turbulence-chemistry interaction

Turbulence enhances mixing, promoting reactivity. Reactions change the temperature, affecting the flow: the **Combustion Model**

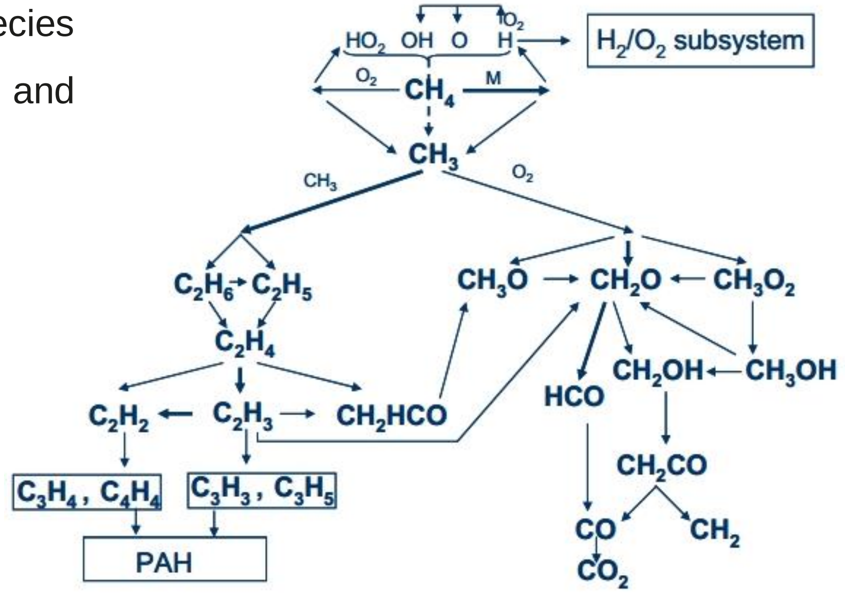
- System configuration + phenomena (flow vs reaction) time scales
  - ✓ MILD combustion: reactants dilution with flue gases, strong chemistry-fluid dynamics competition (Da≈1)
  - ✓ Industrial system: description of slow-forming species (NOx)
- Non-premixed combustion + Finite Rate approach
- EDC + Partially Stirred Reactor (PaSR) model
  - ✓ Specific for MILD combustion: domain-variable interaction parameters based on local conditions (Da)



	Premixed Combustion	Non-Premixed Combustion	Partially Premixed Combustion
Fast Chemistry	Premixed Combustion Model Reaction Progress Variable	Non-Premixed Equilibrium Model Mixture Fraction	Partially Premixed Model Reaction Progress Variable + Mixture Fraction
Fast Chemistry		Laminar Diffusion Flamelet Model (Steady/Unsteady)	
Fast Chemistry	Flamelet Generated Manifold Model		
Fast Chemistry	Finite Rate/Eddy Dissipation Model		
Finite Rate Chemistry	Laminar Finite Rate Model		
Finite Rate Chemistry	Eddy-Dissipation Concept (EDC) Model		
Finite Rate Chemistry	Composition PDF Transport Model (Eulerian/Lagrangian)		

Kinetic Mechanism

Must reproduce the oxidation the fuels and of all the relevant sub-species alongside the whole temperature range experienced in the system (CH_4, H_2 and all their mixtures). MILD combustion: intermediate species are important!



Complexity / Accuracy / CPU time

- **Global kinetic mechanisms**: not suggested for MILD
- **Skeletal**: ok within the validity range
  - ✓ KEE58: suitable, but NOx sub-mech is missing
- **Detailed**: suggested for MILD, but a limited number of species (~50, calculation time)
  - ✓ Accurate description of radical species (MILD combustion)
  - ✓ NOx: required, one of the burner design target and benchmark at industrial level

Name	Type	Species	Reactions	NOx sub-mech.
KEE58	Skeletal	17	58	No
GRI211	Detailed	49	279	Yes
GRI30	Detailed	53	325	Yes
POLIMIC1C3HT_NOx	Detailed	159	2459	Yes

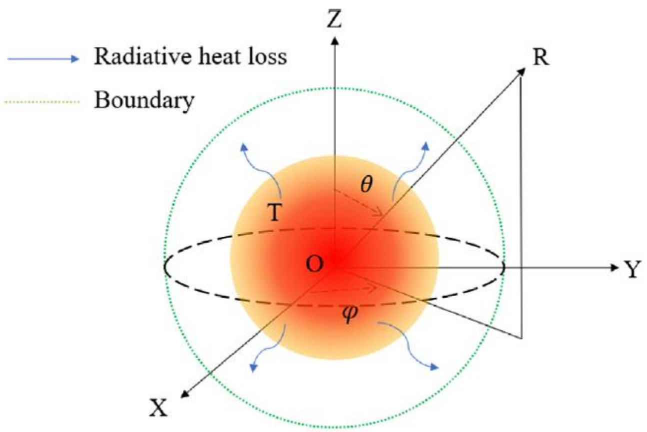
Radiation

RADIATIVE TRANSFER EQUATION

Radiative Transfer Equation (RTE): spatial evolution of radiative intensity I and the interaction with surroundings

Complexity / Accuracy / CPU time

- **Monte Carlo (MC)**
  - ✓ Random ray tracing to simulate photons path/interactions with surfaces
  - ✓ Complex geometries, non-uniform media and spectrally-dependent properties
- **Discrete Ordinate (DO)**
  - ✓ FVM discretization of RTE
  - ✓ Optically thin media
- **P1**
  - ✓ Projection of I using set of spherical harmonics (avg + 1st)
  - ✓ Optically thick media + no significant wall emissions



Zheng et al., ES Energy Environ., 2021, 12, 4-45

Radiation

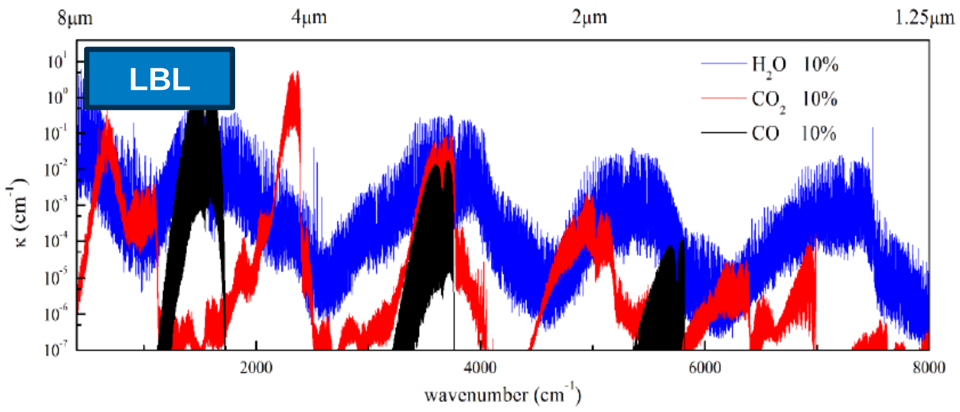
GAS EMISSIVITY MODEL

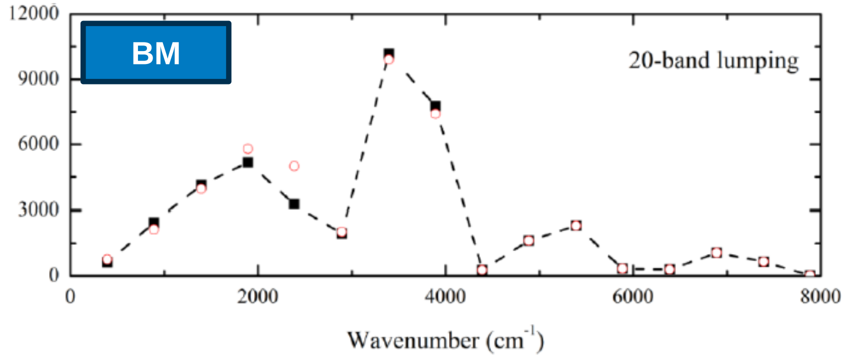
From CH_4 to H_2: combustion atmosphere composition change, affecting radiation phenomena.

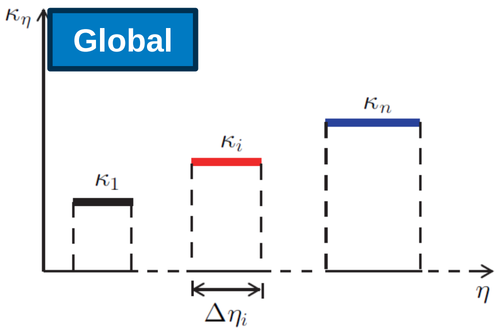
- Total gas emissivity $\varepsilon = f(k_i)$: solving 1 RTE at given T for each wavenumber η, and for each species. Repeat for each T
  - ✓ Very demanding computation!

Complexity / Accuracy / CPU time

- **Line-By-Line (LBL) Models:** 0.01 cm^{-1} sampling
- **Band Models (BMs):** 10-1000 cm^{-1} sampling
- **Global Models:** average value(s)
  - ✓ WSGGM: weighted sum of grey gases
  - ✓ Grey Gas: single grey gas







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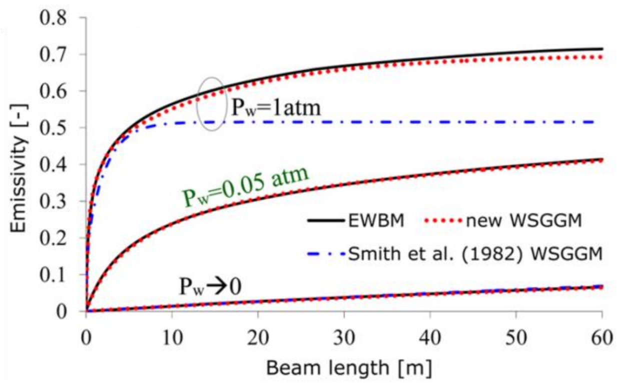
Radiation

WSGG MODEL

WSGGM: composition effects described by averaging the emissivity of 3 grey gases + 1 transparent (non-grey behavior of real gases). Temperature-dependence: fitting coefficients a_i

$$\varepsilon = \sum_{i=0}^{N} a_i(T)(1 - e^{-k_i PXL})$$

- **Smith et al.**
  - ✓ Most common in CFD codes
  - ✓ $600 \leq T \leq 2400\ K,\ P_{H_2O}/P_{CO_2} = 1, 2,\ 0.001 \leq L \leq 10\ m$
- **Yin et al.**
  - ✓ $600 \leq T \leq 2400\ K,\ P_{H_2O}/P_{CO_2} = 0.125{:}\,4,\ 0.001 \leq L \leq 60\ m$
  - ✓ Extension toward combustion atmospheres with high H_2O + industrial-sized equipment
- Depending on the case, the model by Smith et al. is suitable also with H_2
  - ✓ Significant differences for pure water atmospheres + L>10m
  - ✓ No significant differences at lab-scale cases (L~1 m)



	Tgas avg [°C]	Tgas max [°C]	ε avg [1/m]	ε max [1/m]
Smith et al.	1139	1625	0.241	0.256
Yin et al.	1138	1617	0.264	0.288

Yin, Energy & Fuels, 2013, 27,10

Smith et al., Jurnal of Heat Transfer, 1982, 104, 4.

Tenova TLX Burner

CFD ANALYSIS

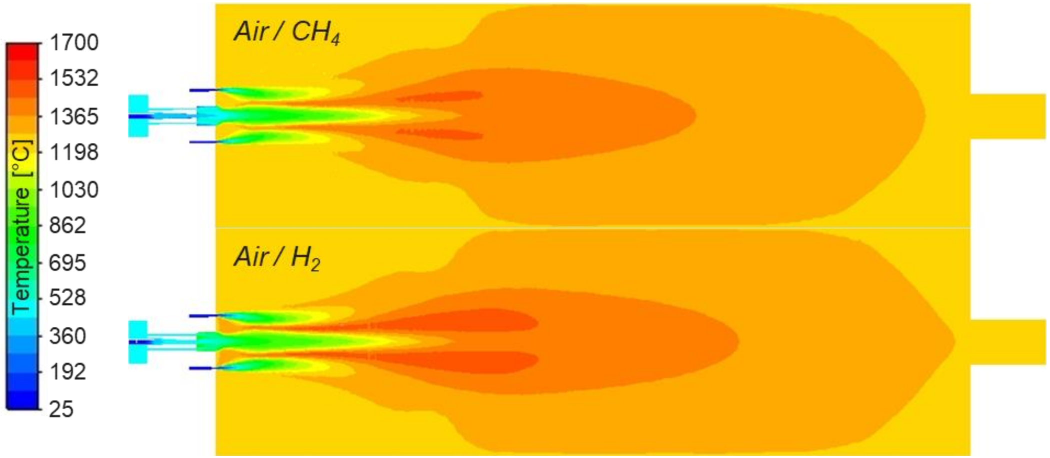
- Tenova TLX burner performance assessment with CH_4 and H_2
  - ✓ Experimental data available in the next future (preliminary design)

HyTecHeat

- Diffuse combustion, very uniform temperature field
- H_2 combustion
  - ✓ Increased reactivity: extended core zone
  - ✓ Flameless technology: no significant temperature increase
- Emissions aligned with other Tenova "H_2 Ready" burners

Furnace Exit	Air/CH_4	Air/H_2
Temperature [°C]	1269	1272
O_2 [%mol]	1.1	1.3
NOx 3% O_2 [ppm]	33	16

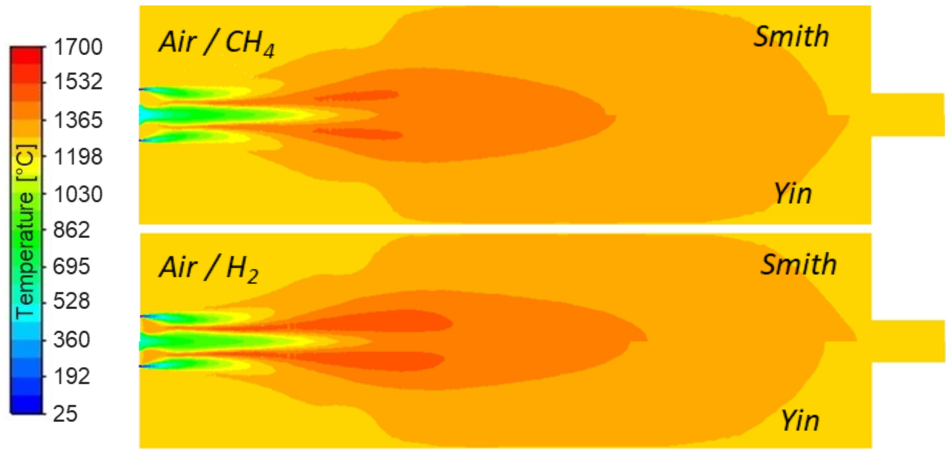
Tenova TLX	
Power [kW]	320
Fuel	CH_4, H_2 and mixtures
Air Temperature [°C]	450
Furnace Temperature [°C]	1250



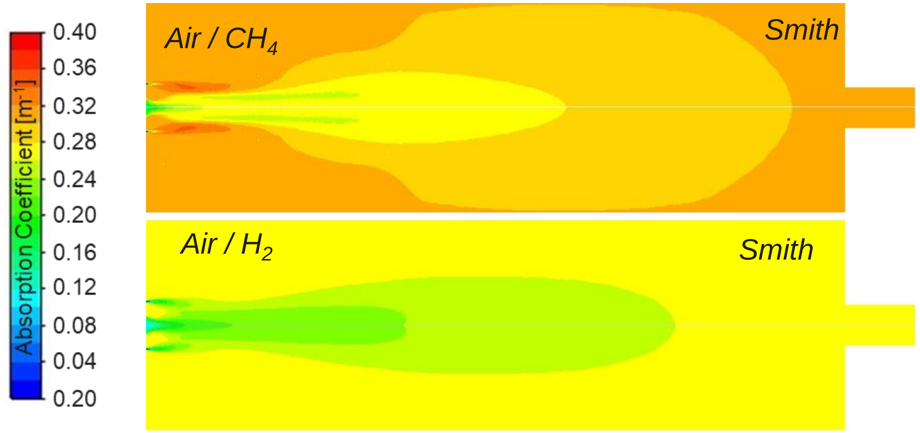
Tenova TLX Burner

RADIATION MODEL COMPARISON

- WSGGM model: Smith et al. vs Yin et al.
  - ✓ Flame structure, temperature distribution and wall heat fluxes are not affected
  - ✓ Expected higher discrepancies in combustion atmospheres with higher H_2O + industrial-size equipment
- H_2 combustion: increased wall heat flux
  - ✓ Different CO_2/H_2O ratio: lower absorption coefficient



Average Data		Air/CH_4	Air/H_2
Peak Temperature [°C]	Smith et al.	1491	1491
	Yin et al.	1491	1491
Furnace Exit Temperature [°C]	Smith et al.	1269	1272
	Yin et al.	1272	1268
Mean ε [m^{-1}]	Smith et al.	0.30	0.27
	Yin et al.	0.27	0.32
Total Wall Radiation Heat Flux [kW]	Smith et al.	40.8	45.3
	Yin et al.	40.5	45.8



Conclusion

- A CFD model for the simulation of a flameless burner running with any CH_4/H_2 mixture was successfully developed and applied to the simulation of the Tenova TLX burner
- The analysis confirms the target performances of the Tenova TLX burner
  - ✓ Flameless technology enables the use of H_2 in the steel sector: temperature and emissions control
  - ✓ Unifor temperature distribution, low NOx emissions (in-line with other Tenova “Hydrogen Ready” burners)
- The WSGGM model of Smith et al. can be used also in these specific cases
  - ✓ Lab-scale combustion chamber (low beam length) and low water content
  - ✓ Higher water content / Industrial-size equipment: more general models required
- Some open points
  - ✓ Reliable measurement systems for combustion atmospheres with high vapor content
  - ✓ Models enabling full-furnace simulation with reasonable time (kinetic mechanisms, combustion models, pollutant estimation, etc.)

Acknowledgments

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OUR COMMITMENT TOWARD A CLEANER FUTURE

European Commission

Research Fund for Coal & Steel

Acknowledgements: The research leading to these results has received funding from the European Union's Research Fund for Coal and Steel research program under grant agreement number 101092087

NOx

CO_2

4.0

HyTecHeat

H_2ReUse

Life

NOxRF (2003-07)	***CO2RED*** *(2006-10)*	***BURNER4.0*** *(2019-23)*	***HyTecHeat*** *(2022-25)*	***H2REUSE*** *(2023-26)*
Primary NOx reduction by testing and modelling flameless low NOx burners both high temperature air and oxy combustion	**New combustion technology** allowing a step change in environmental impact of reheating furnaces (CO_2 and NOx)	**Industry 4.0 enabling technologies** applied to the best available combustion system for better performance and reliability of furnace	**Hybrid heating technology** (progressive and increasing H2 usage) in downstream processes	**Highly efficient and sustainable decarbonization** of bright annealing process by recovery and reuse of H_2

THANK YOU


GREEN SOLUTIONS
FOR DECARBONIZATION AND SUSTAINABLE TECHNOLOGIES FOR METALS
Tenova Hydrogen Technologies
Heating Strategies towards Decarbonization
Tenova Combustion Technologies