Computational fluid dynamics-based study of novel technologies in steam cracking furnaces

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IMPROOF

Introduction to steam cracking

Hydrocarbon feed is cracked at high temperatures to produce light olefins

IMPROOF objective

Improve the energy efficiency of the steam cracking process

Reactor side

- 3D reactor technologies

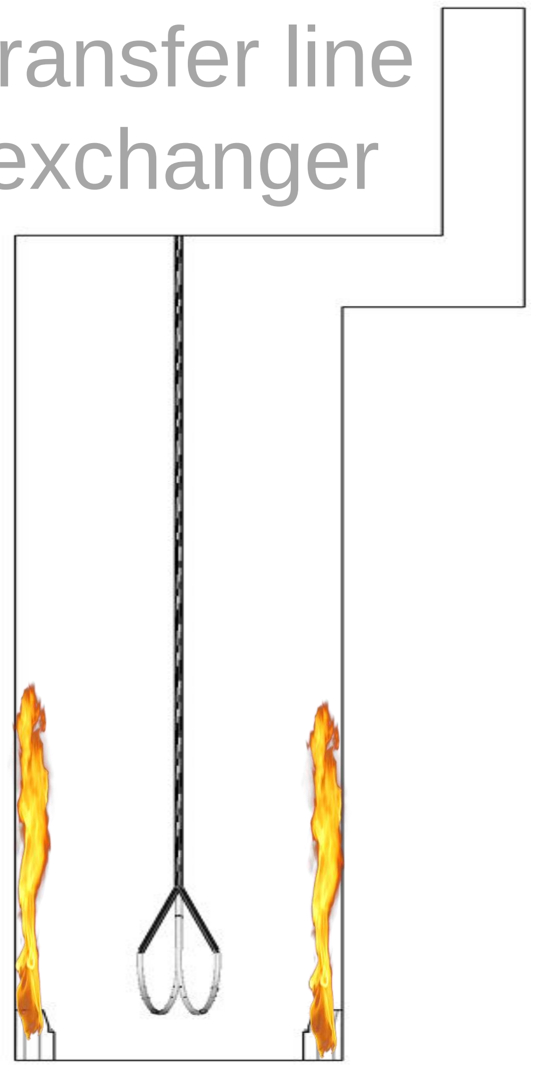
Furnace side

- high emissivity coatings
- oxy-fuel combustion

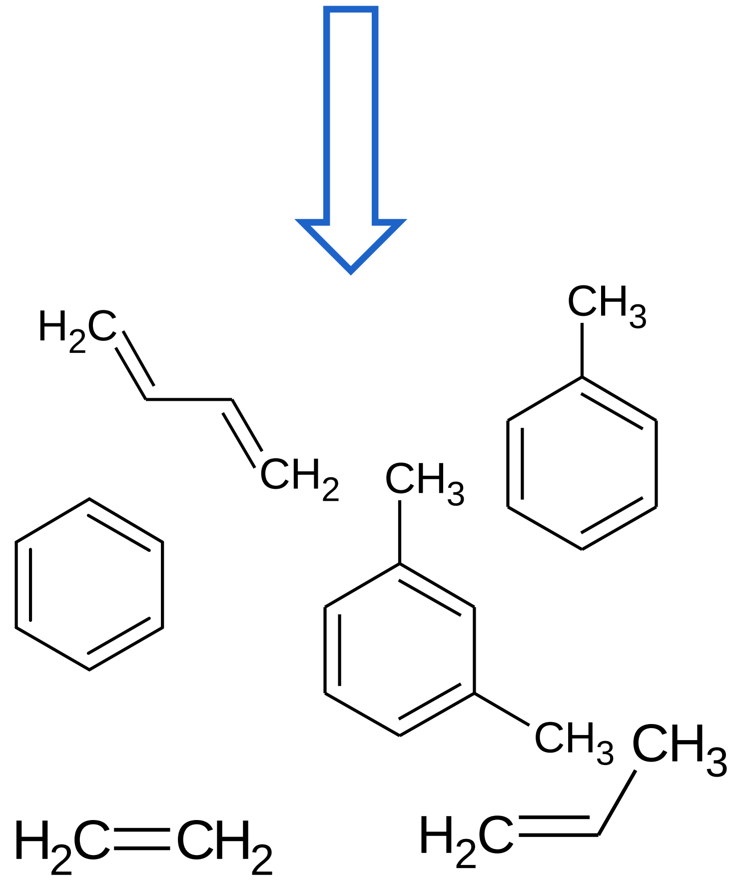
Convection section

Transfer line exchanger

Radiant section



Hydrocarbon feed



Commodity chemicals

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Reactor side

3D reactor technologies

Furnace side

High emissivity coatings

Oxy-fuel combustion

Reactor side

3D reactor technologies

Furnace side

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Oxy-fuel combustion

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3D reactor technologies

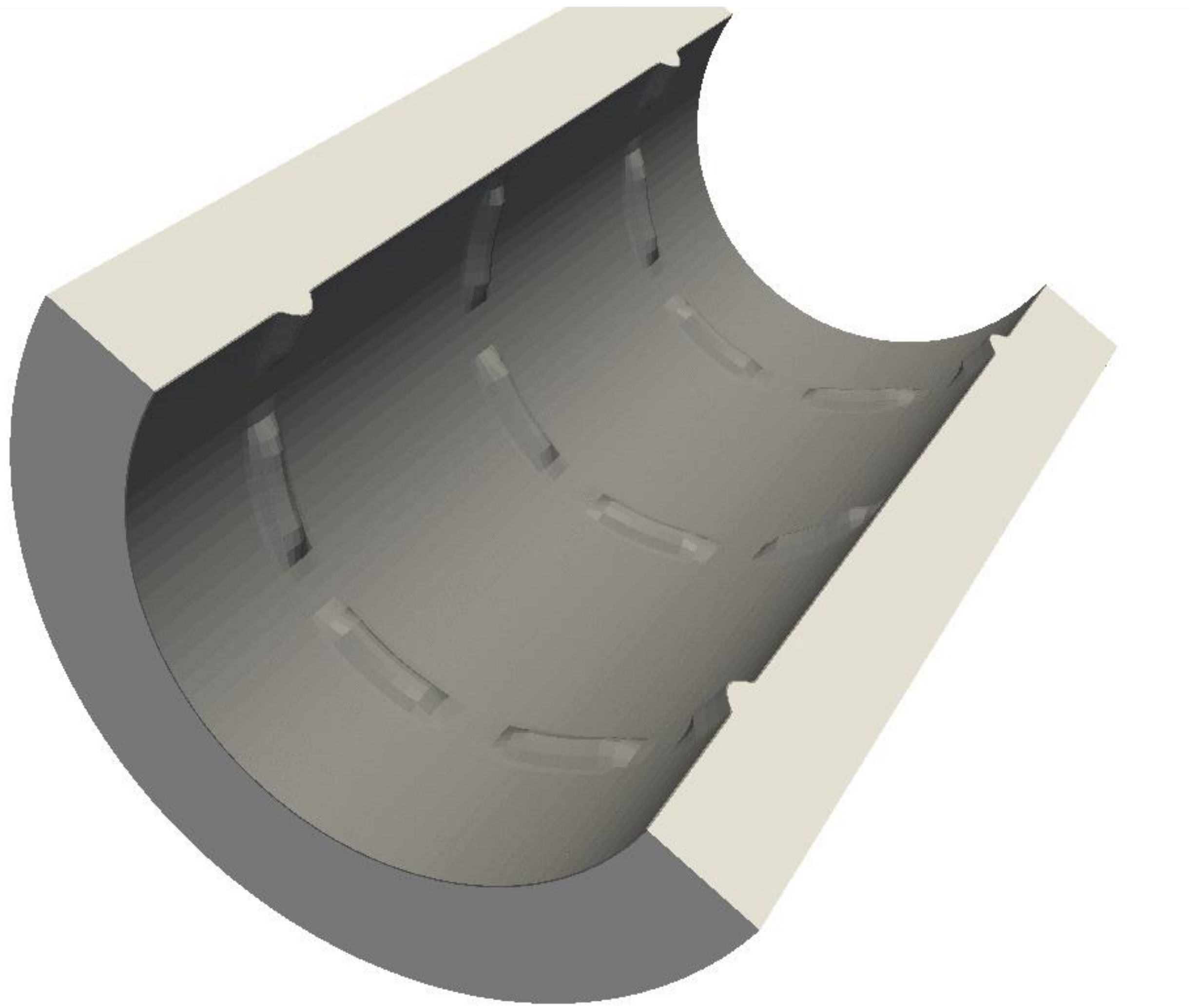
Coke: deposition of a carbon residue layer on the reactor surface

thermal efficiency ↓

product selectivity ↓

decoking procedures required

→ Nemesis of the steam cracking process



Optimization by:

- feed additives
- metallurgy & surface technologies
- 3D reactor technologies

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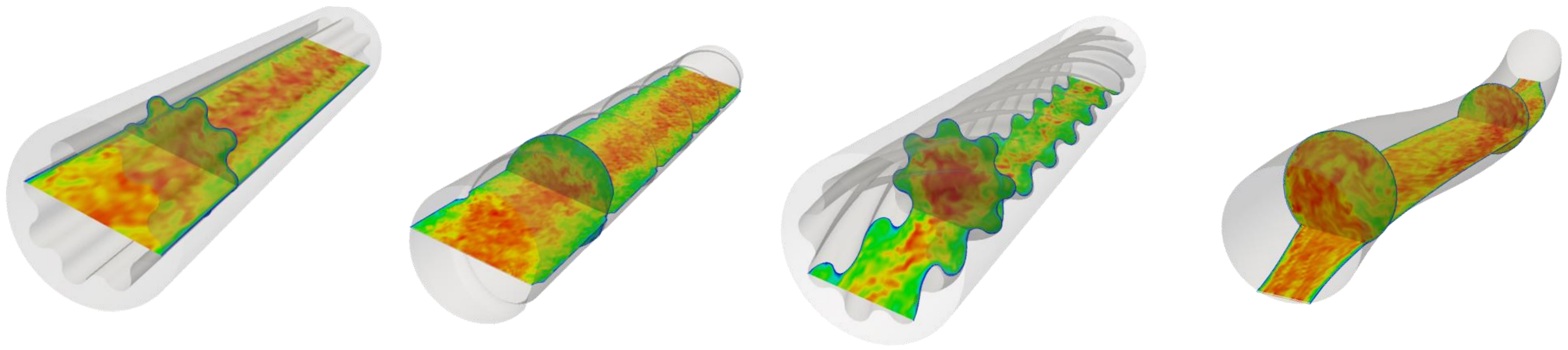
[1] Vandewalle, L. A.; Van Cauwenberge, D. J.; Dedeyne, J. N.; Van Geem, K. M.; Marin, G. B., Dynamic simulation of fouling in steam cracking reactors using CFD. *Chemical Engineering Journal* **2017**.

3D reactor technologies

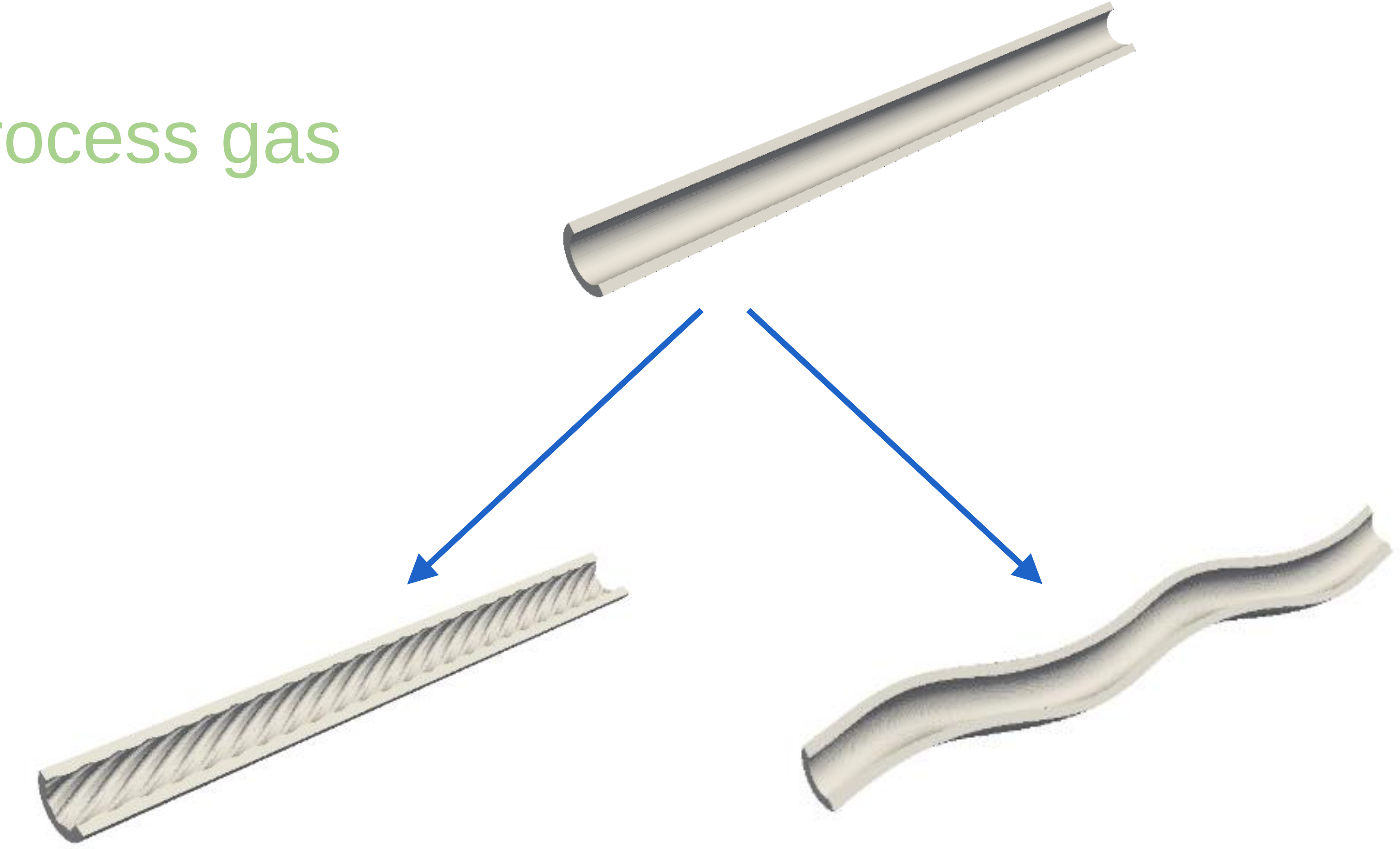
$$Q_{net} = U\,A\left(T_{reactor\,wall} - T_{fluid}\right)$$



Process intensification?

$A \uparrow$ more reactor material needed

$U \uparrow$ improve heat transfer from metal to process gas



3D reactor technologies

Decrease temperature boundary layer

Increase radial mixing

Increased pressure drop

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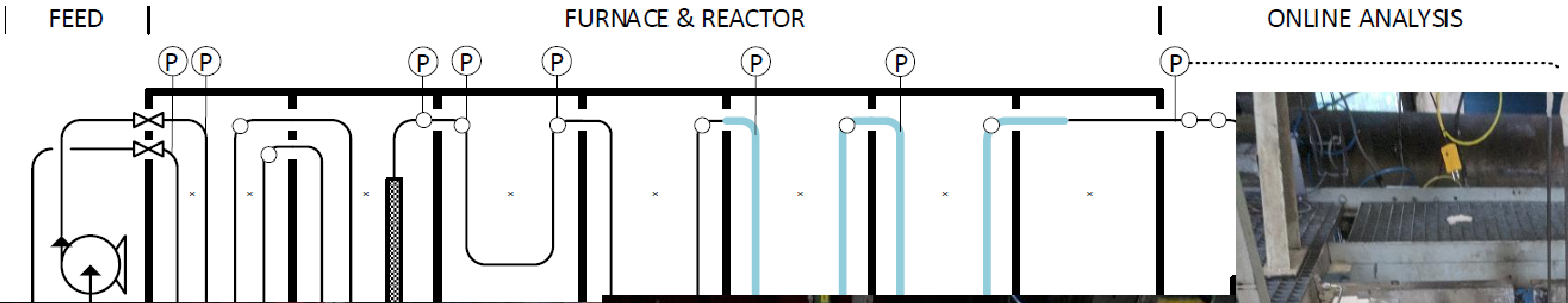
[2] Van Cauwenberge, D. J.; Schietekat, C. M.; Floré, J.; Van Geem, K. M.; Marin, G. B., CFD-based design of 3D pyrolysis reactors: RANS vs. LES. *Chemical Engineering Journal* **2015**.

Steam cracking pilot plant experiments



Operating conditions:

mperature
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rogram:

(CCs)
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O)

D_i: 9

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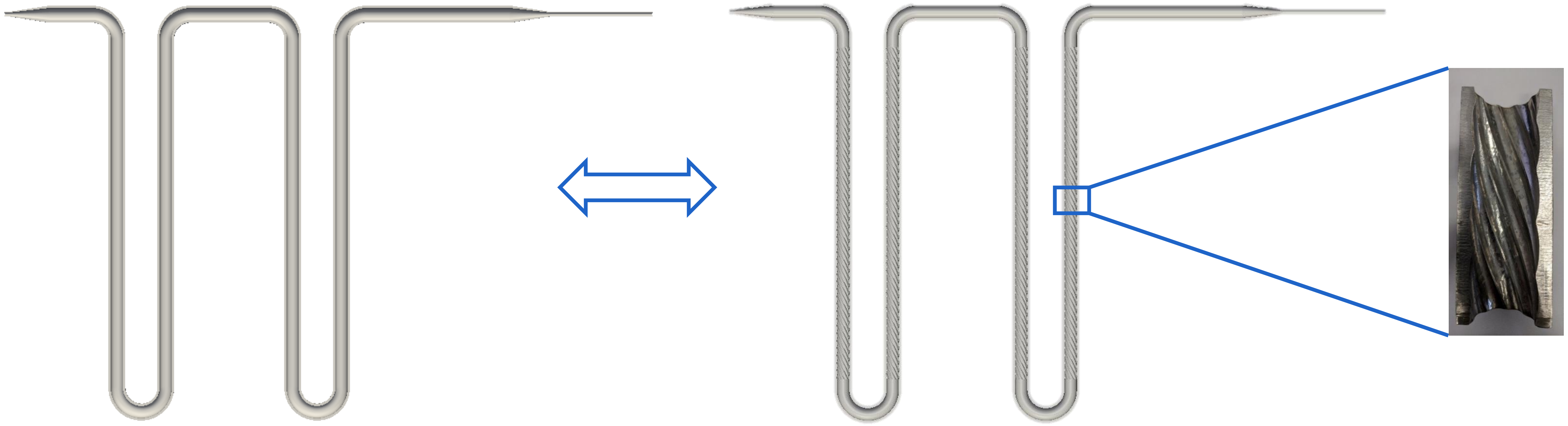
Steam cracking pilot plant CFD

reactive Reynolds-averaged Navier-Stokes CFD simulation

k-omega SST turbulence model

Effect of 3D reactor technologies on a pilot plant scale?



CFD simulations running…

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Reactor side

3D reactor technologies

Furnace side

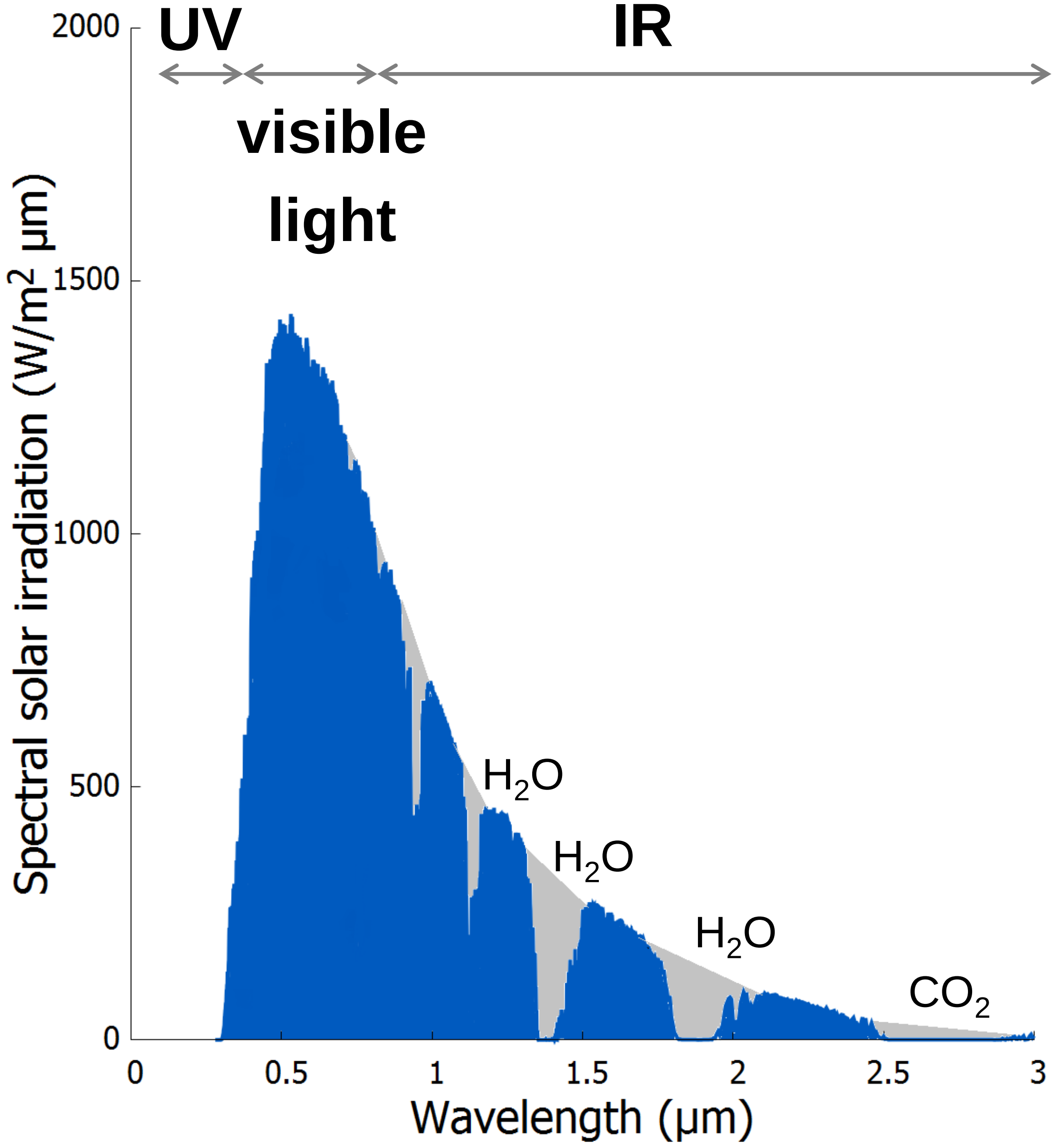
High emissivity coatings

Oxy-fuel combustion

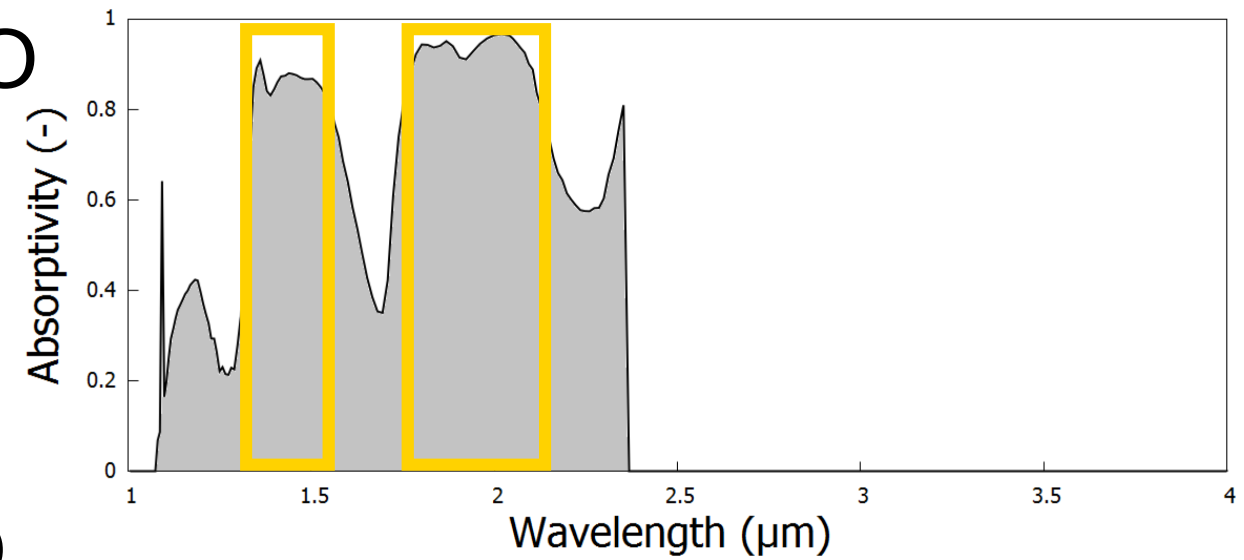
Introduction radiative heat transfer

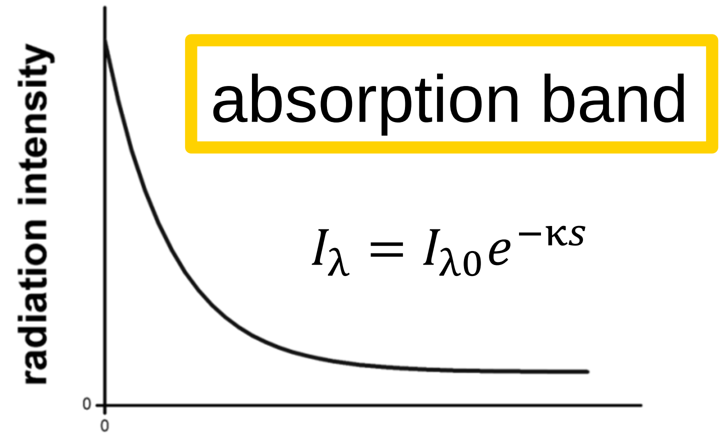
Solar spectrum as the primary source of renewable energy:

- spectrum resembles that of a 5800 K blackbody
- gas phase absorption due to gases in atmosphere

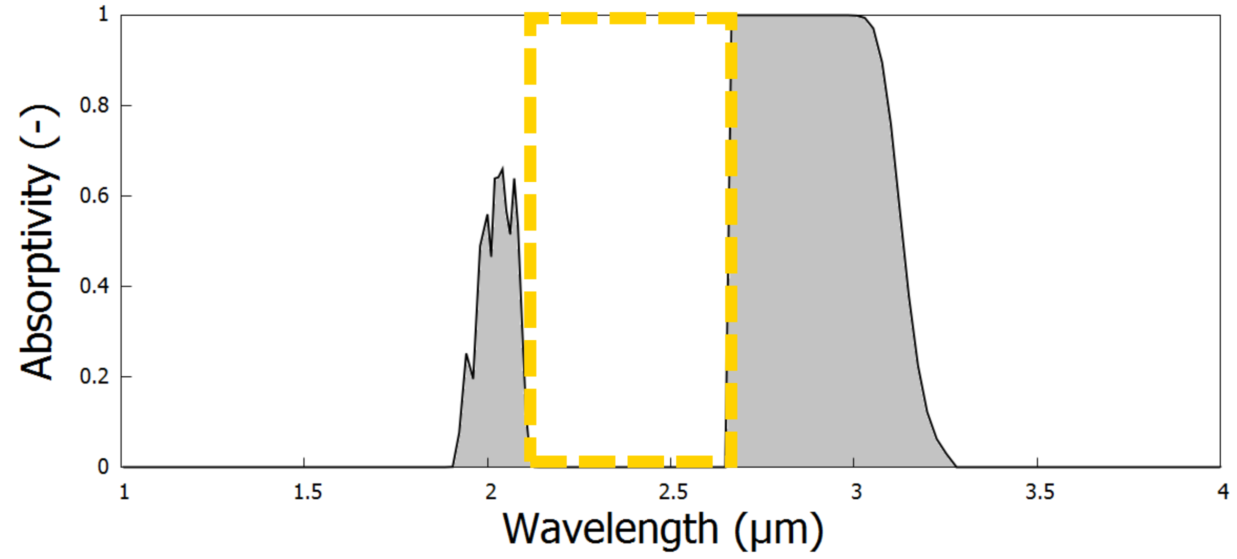


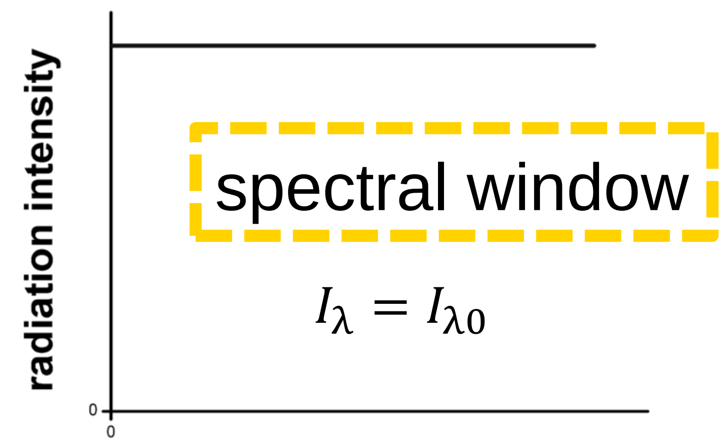
H_2O





CO_2





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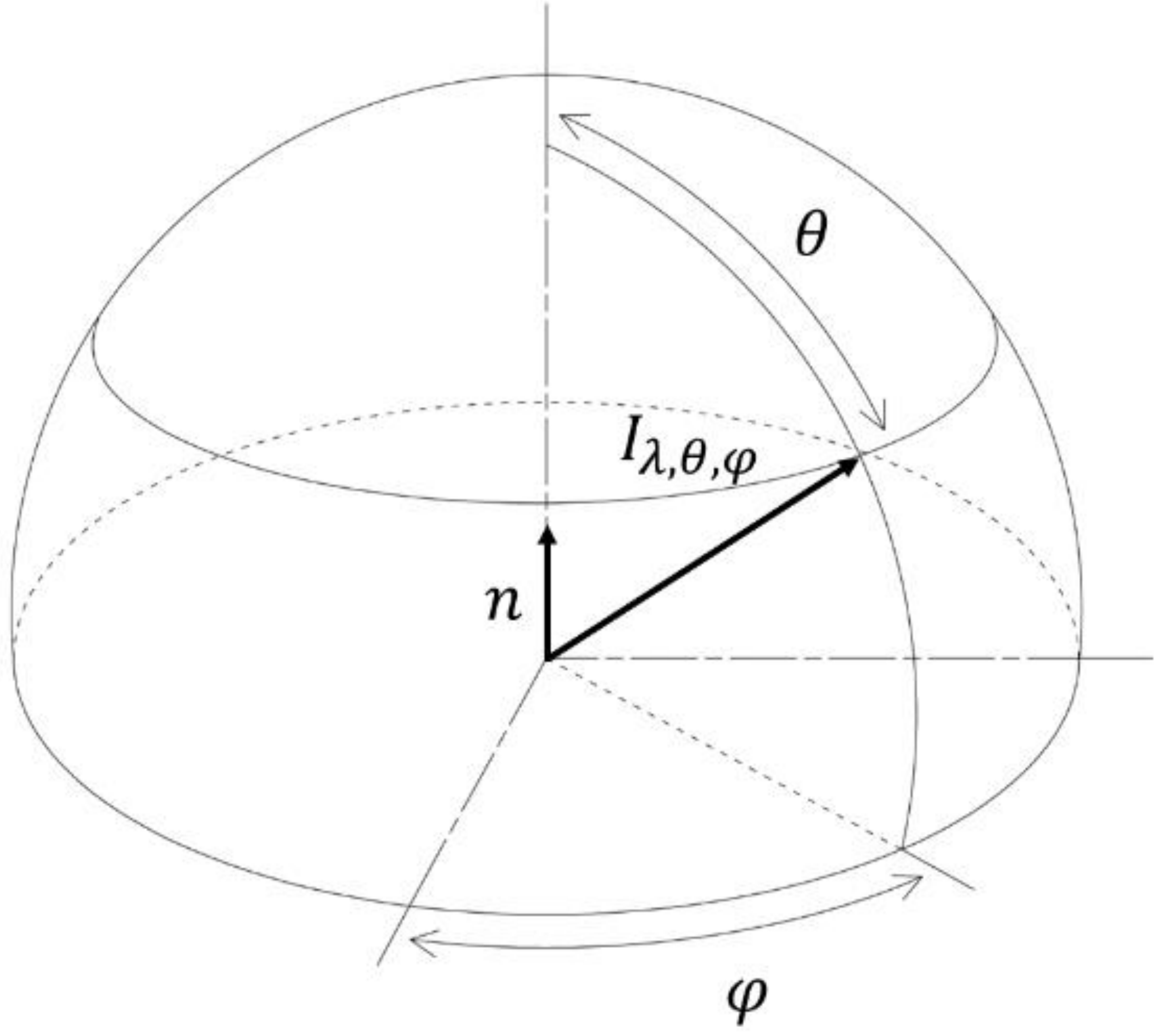
[2] Reference Solar Spectral Irradiance: ASTM G-173. Available at: ⟨http://rredc.nrel.gov/solar/spectra/am1.5⟩, (accessed 26.02.18).
[3] Reference NIST RADCAL Narrow-Band model developed by W. Grosshandler. Updated version available at: ⟨ https://github.com/firemodels/radcal ⟩, (accessed 20.02.18).

Spectral directional emissivity

No object behaves as a perfect blackbody → the emissivity is a measure for the deviation of the surface irradiance from a perfect blackbody

The most fundamental emissive property is the *spectral directional* emissivity:

$$\varepsilon_{\lambda,\theta,\varphi}(\lambda,\theta,\varphi,T) = \frac{I_{\lambda,\theta,\varphi}(\lambda,\theta,\varphi,T)}{I_{\lambda}^{B}(\lambda,T)}$$



depends on:
wavelength, polar coordinates, surface conditions…

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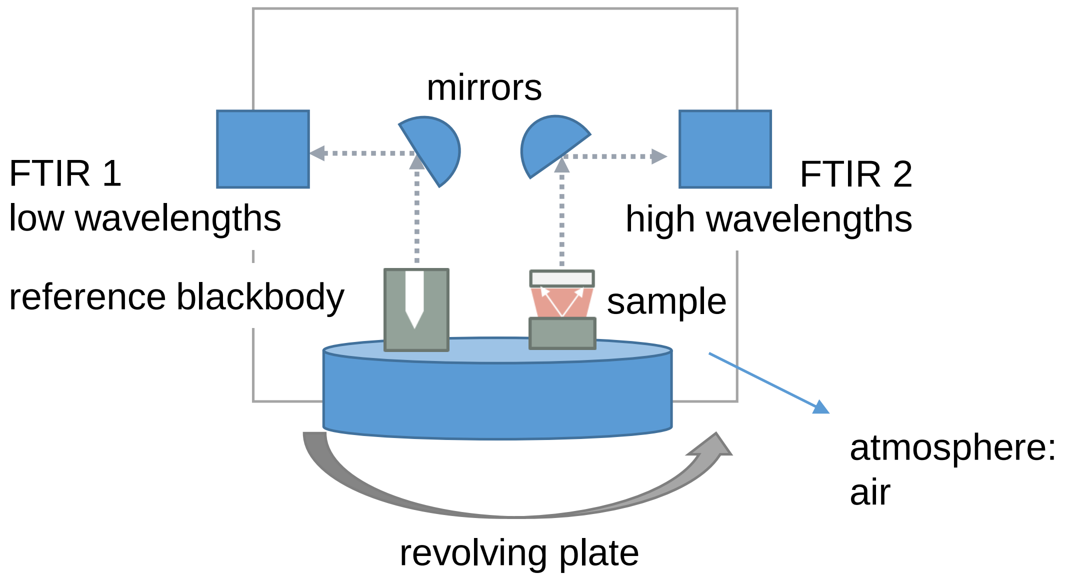
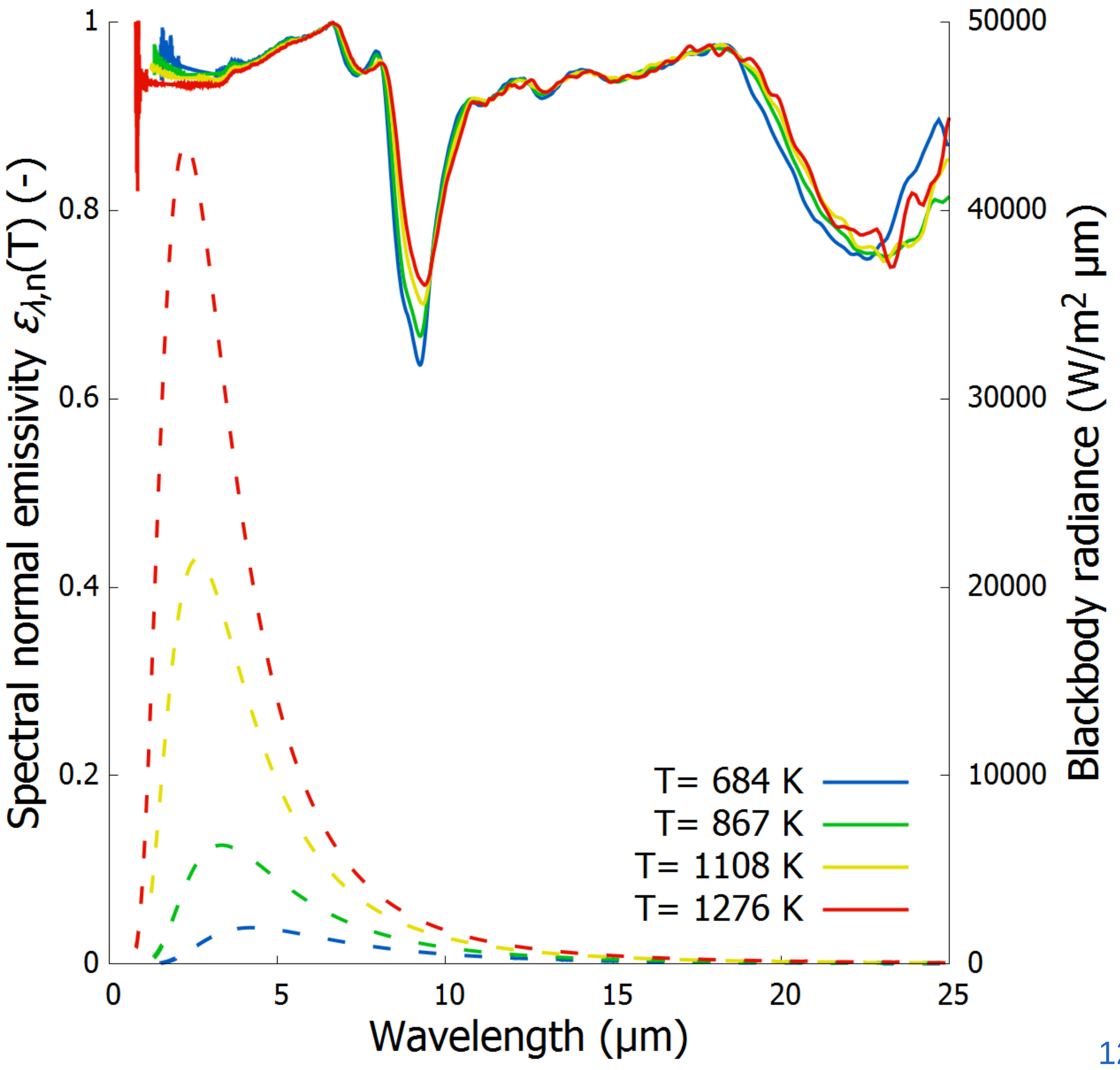
Experimental emissivity characterization

CNRS-CEMHTI: *spectral normal* emissivity measurement device

Emisshield coating:

$$\varepsilon_{\lambda,n}(\lambda,T) = \varepsilon_{\lambda,\theta=0°,\varphi=0°}(\lambda,T) = \frac{I_{\lambda,n}(\lambda,T)}{I_\lambda^B(\lambda,T)}$$





[4] Brodu, E. et al., Reducing the temperature of a C/C composite heat shield for solar probe missions with an optically selective semi-transparent pyrolytic boron nitride (pBN) coating. *Carbon* **2015**.

Modelling radiation

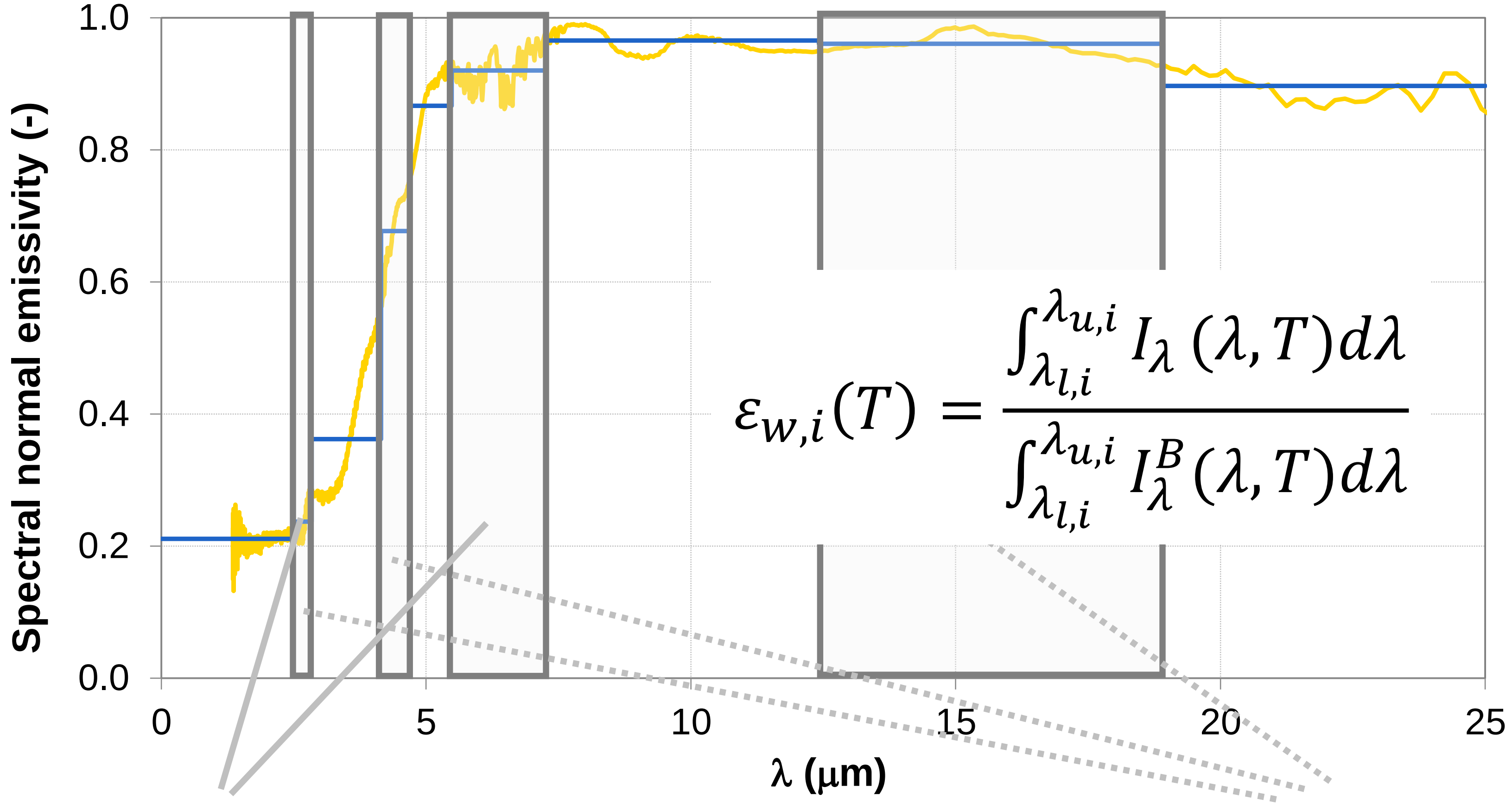
Discrete ordinates model

$$\nabla \cdot (I_i(\vec{r},\vec{s})\vec{s}) + \kappa_i I_i(\vec{r},\vec{s}) = \kappa_i I_{b,i}$$

I_i: spectral intensity
$I_{b,i}$: blackbody spectral intensity
κ_i: absorption coefficient

Exponential wide band model to account for gas phase absorption

Band number	Lower limit (µm)	Upper limit (µm)	Gas phase absorptivity	Wall emissivity
1	0	2.50	0	$\varepsilon_{w,1}$
2	2.50	2.84	EWMB	$\varepsilon_{w,2}$
3	2.84	4.15	0	$\varepsilon_{w,3}$
4	4.15	4.69	EWBM	$\varepsilon_{w,4}$
5	4.69	5.48	0	$\varepsilon_{w,5}$
6	5.48	7.27	EWBM	$\varepsilon_{w,6}$
7	7.27	12.42	0	$\varepsilon_{w,7}$
8	12.42	18.92	EWBM	$\varepsilon_{w,8}$
9	18.92	150.00	0	$\varepsilon_{w,9}$

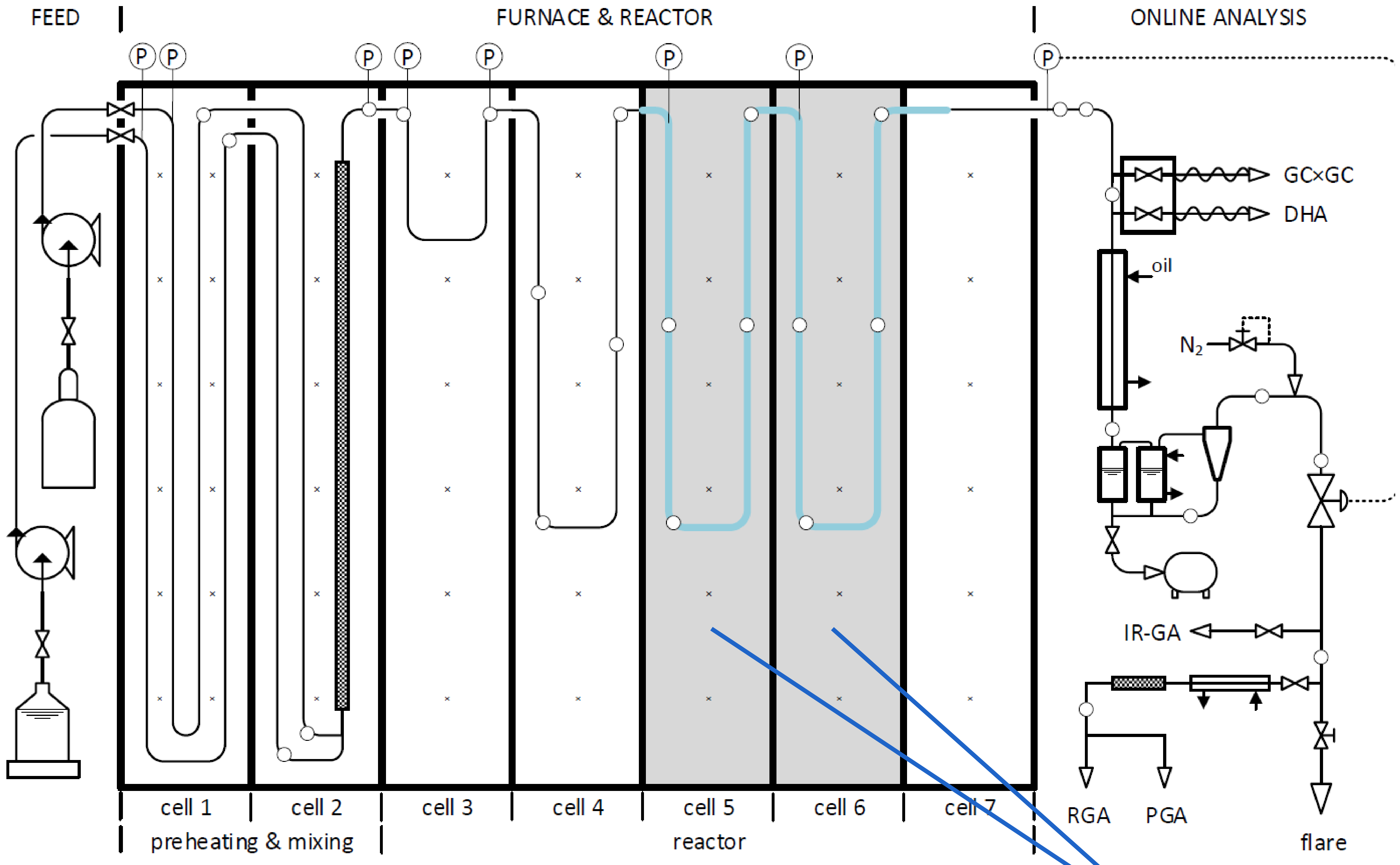


$$\varepsilon_{w,i}(T) = \frac{\int_{\lambda_{l,i}}^{\lambda_{u,i}} I_\lambda(\lambda,T)d\lambda}{\int_{\lambda_{l,i}}^{\lambda_{u,i}} I_\lambda^B(\lambda,T)d\lambda}$$

H_2O absorption bands

model accounts for the boundary wall emissivity and the gas phase absorptivity

Steam cracking pilot plant experiments



D_i: 9 mm D_i: 37.4 mm

high emissivity coating applied on refractory

Operating conditions:
10 kg/h propane
4 kg/h water
644 °C coil inlet temperature
2 bar coil inlet pressure
0.9 s residence time
Re = 4.2 – 5.4 × 10^3
85 % conversion

Experimental program:
Steam treatment
5 cracking cycles (CCs)
decoking after every CC
pre-sulfidation before every CC (300 ppmS H_2O)

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Oxy-fuel combustion

Oxygen is separated from air prior to combustion

Combustion of fuel in the presence of oxygen diluted with recycled flue-gas

→ reduce thermal NO_x emissions

→ concentrated CO_2 flue gas stream easier captured and stored

Future work & connection to workshop: perform CFD simulations in order to reproduce industrial data

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Conclusion

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Conclusion

- 3D reactors offer a way to improve heat transfer from reactor metal to process gas
- High emissivity coatings offer a way to improve energy efficiency of the radiant section of a steam cracking furnace

Future work in the project

- Scale up from pilot scale to industry, a demonstration furnace has been selected
- numerical validation using CFD to confirm the experimental results

Acknowledgments

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IMPROOF

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