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Computational Fluid Dynamics-based Study of the Steam Cracking Process using a Hybrid 3D-1D Approach

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[1]Laboratory for Chemical Technology

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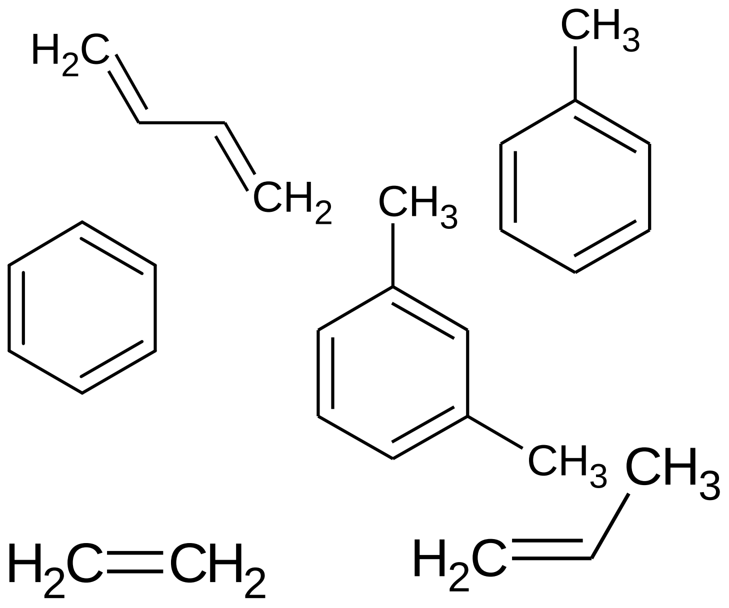
Introduction: the steam cracking process

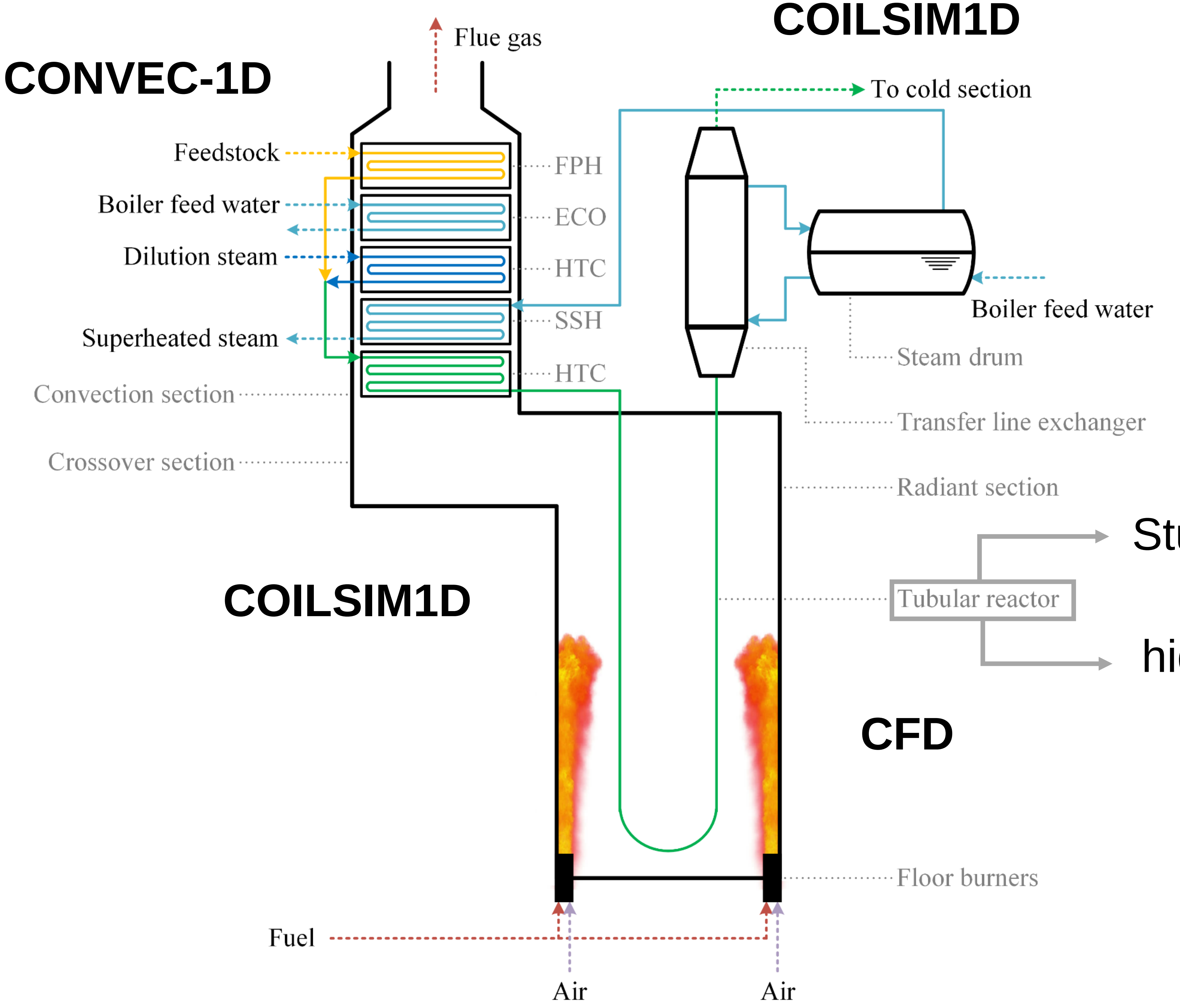
Hydrocarbon feed is cracked at high temperatures to produce light olefins



Commodity chemicals

CONVEC-1D

COILSIM1D



COILSIM1D

Study effect of emissivity

high vs low emissivity

CFD

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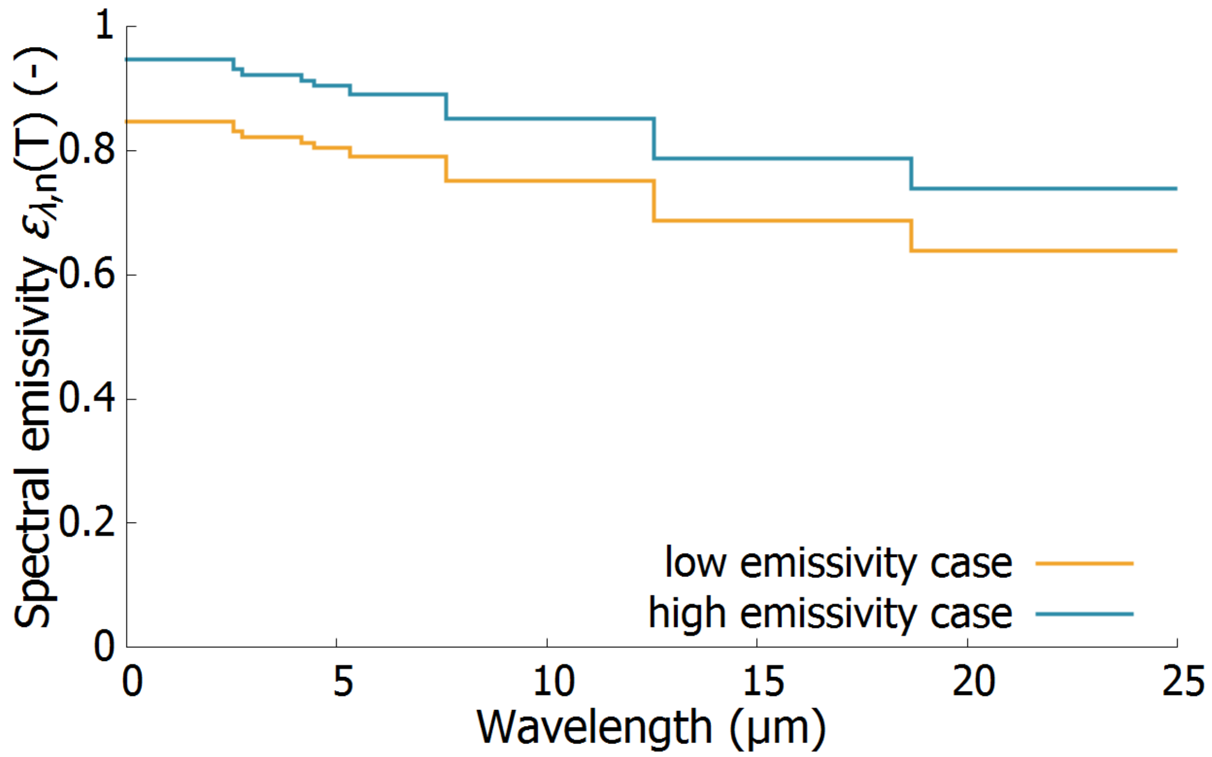
Introduction: emissivity

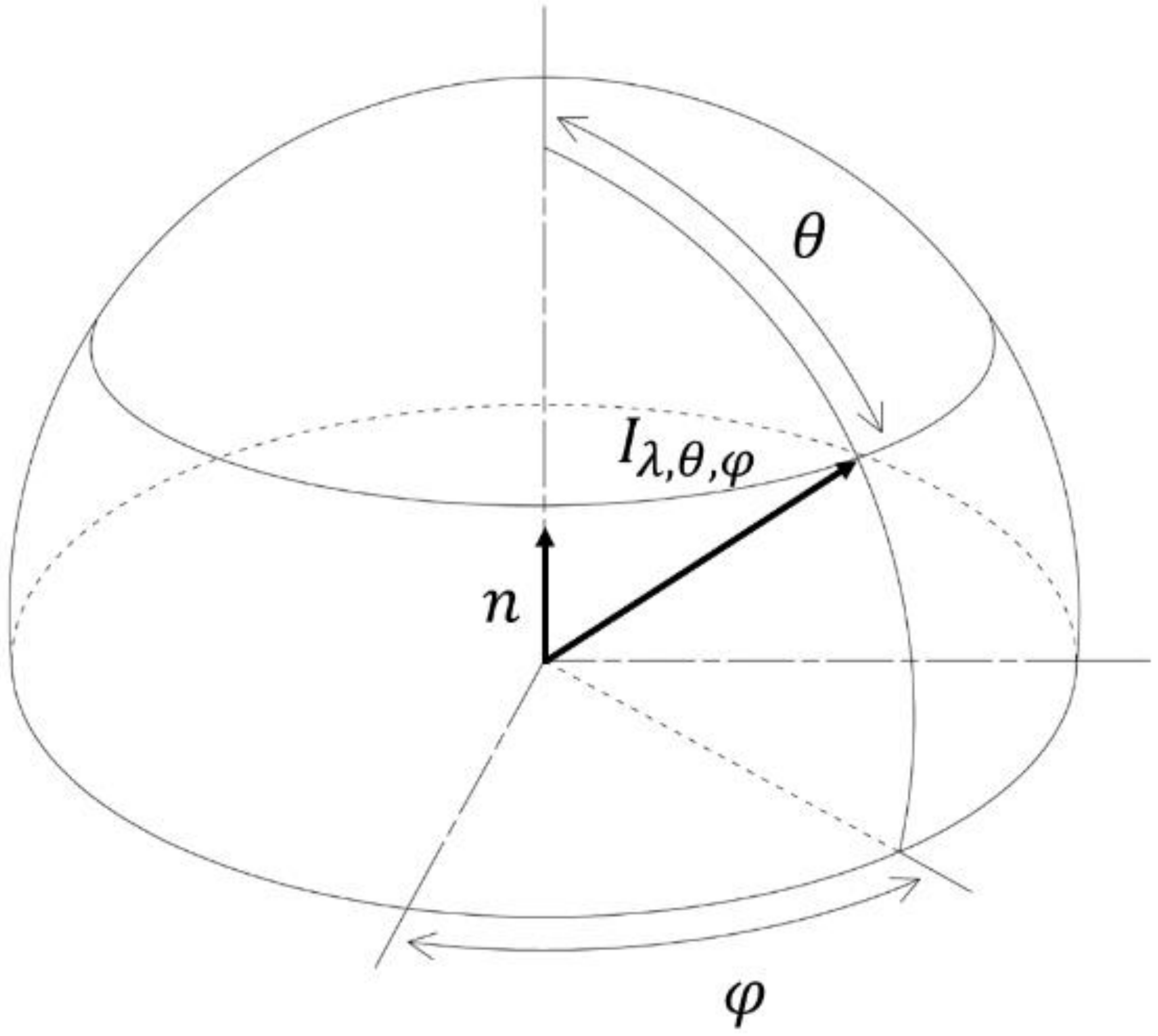
The **emissivity** is a measure for the deviation of the surface irradiance from a perfect blackbody.

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

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

accounting for spectral dependency





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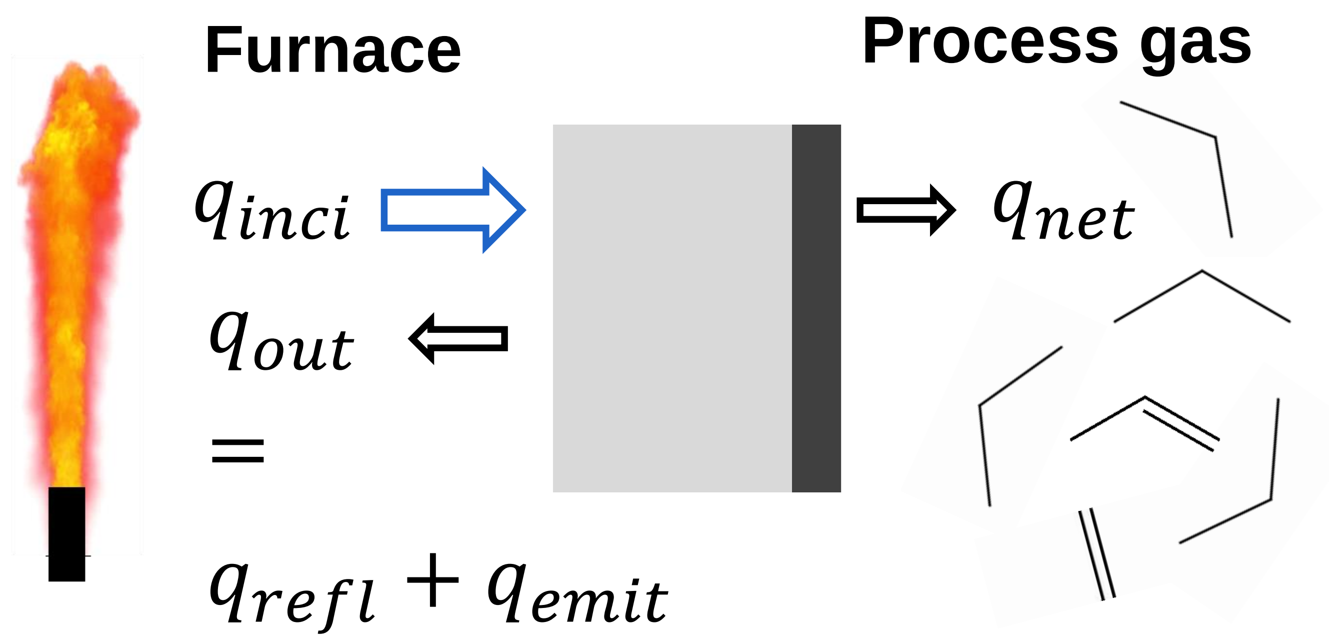
Introduction: radiative heat transfer

Radiative energy balance on a process tube

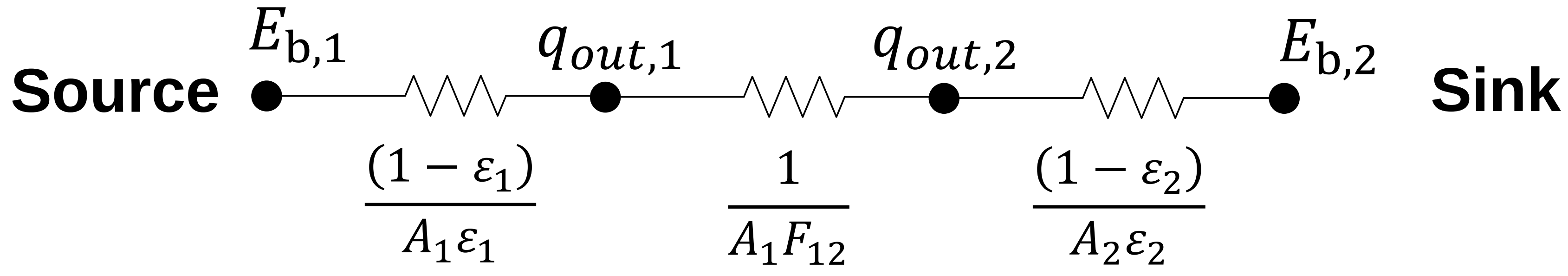
$$q_{inci} = q_{net} + q_{out}$$
$$= q_{net} + q_{refl} + q_{emit}$$
$$= q_{net} + (1-\varepsilon)q_{inci} + \varepsilon\sigma T^4$$



Total heat supplied to process gas

$$Q = A.q_{net} = A[q_{inci} - q_{out}] = A\left[\frac{q_{out} - \varepsilon E_b}{1-\varepsilon} - q_{out}\right] = \frac{q_{out} - E_b}{\left(\frac{1-\varepsilon}{A\,\varepsilon}\right)}$$

This way the "**electric circuit analogy**" can be introduced:



Total heat transfer from source to sink:

$$Q_{1,2} = \frac{E_{b,1} - E_{b,2}}{\frac{(1-\varepsilon_1)}{A_1\varepsilon_1} + \frac{1}{A_1F_{12}} + \frac{(1-\varepsilon_2)}{A_2\varepsilon_2}}$$

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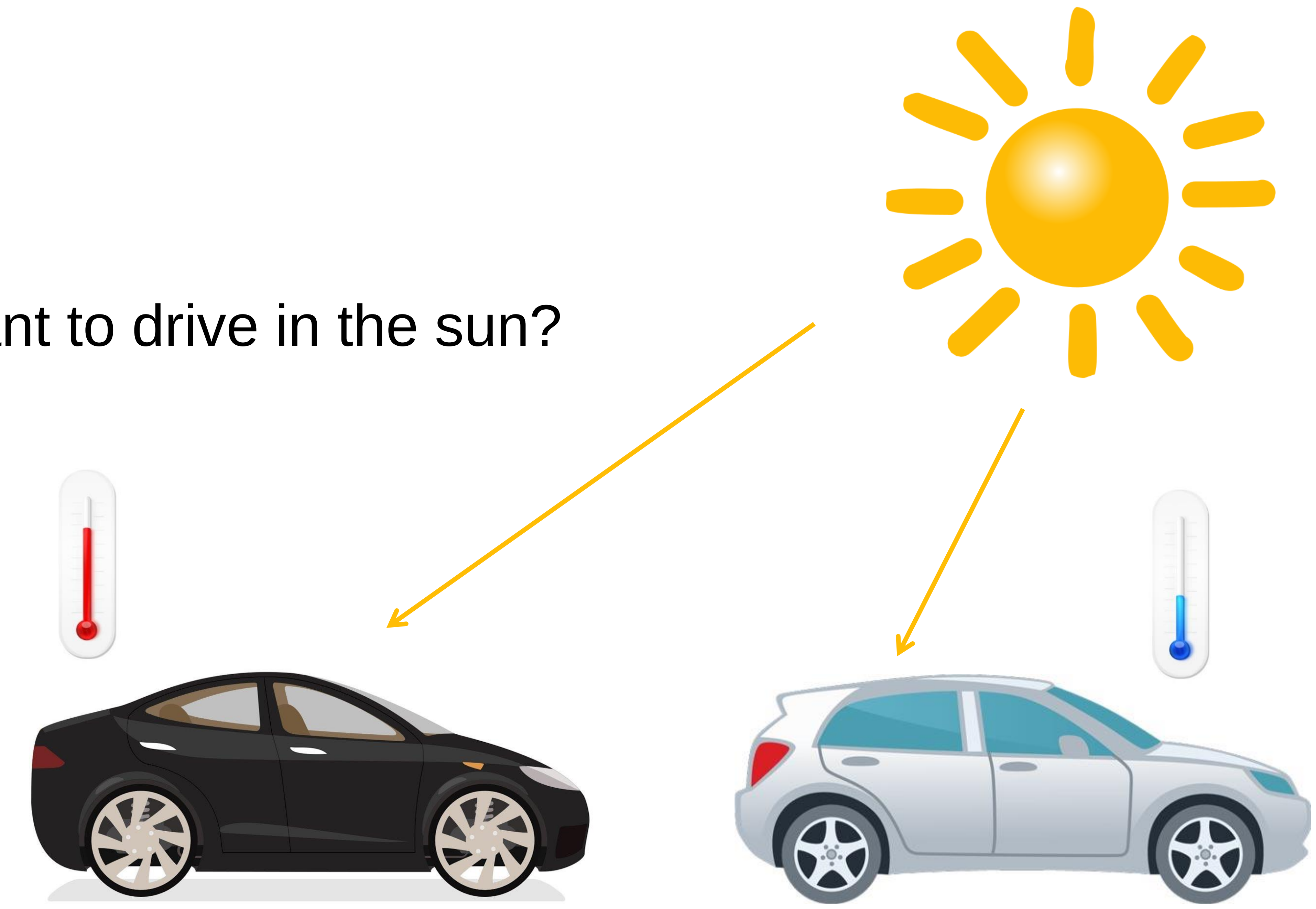
Introduction: absorption

Radiative heat transfer between two surfaces: example

$$Q_{1,2} = \frac{E_{b,1} - E_{b,2}}{\frac{1}{A_1 F_{12}} + \frac{(1-\varepsilon_2)}{A_2 \varepsilon_2}}$$

Which car would you want to drive in the sun?



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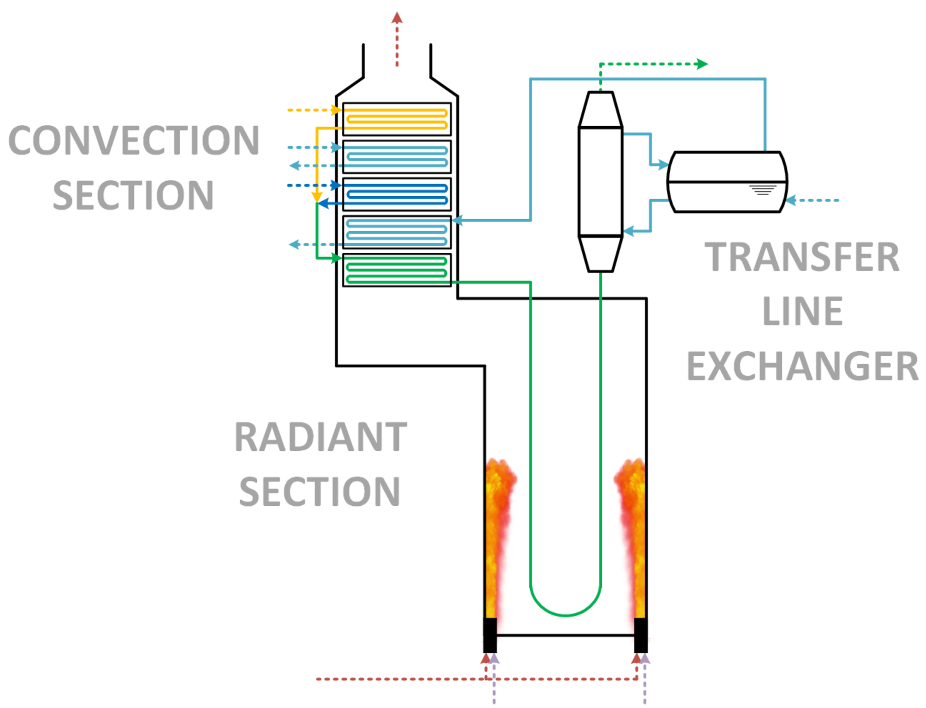
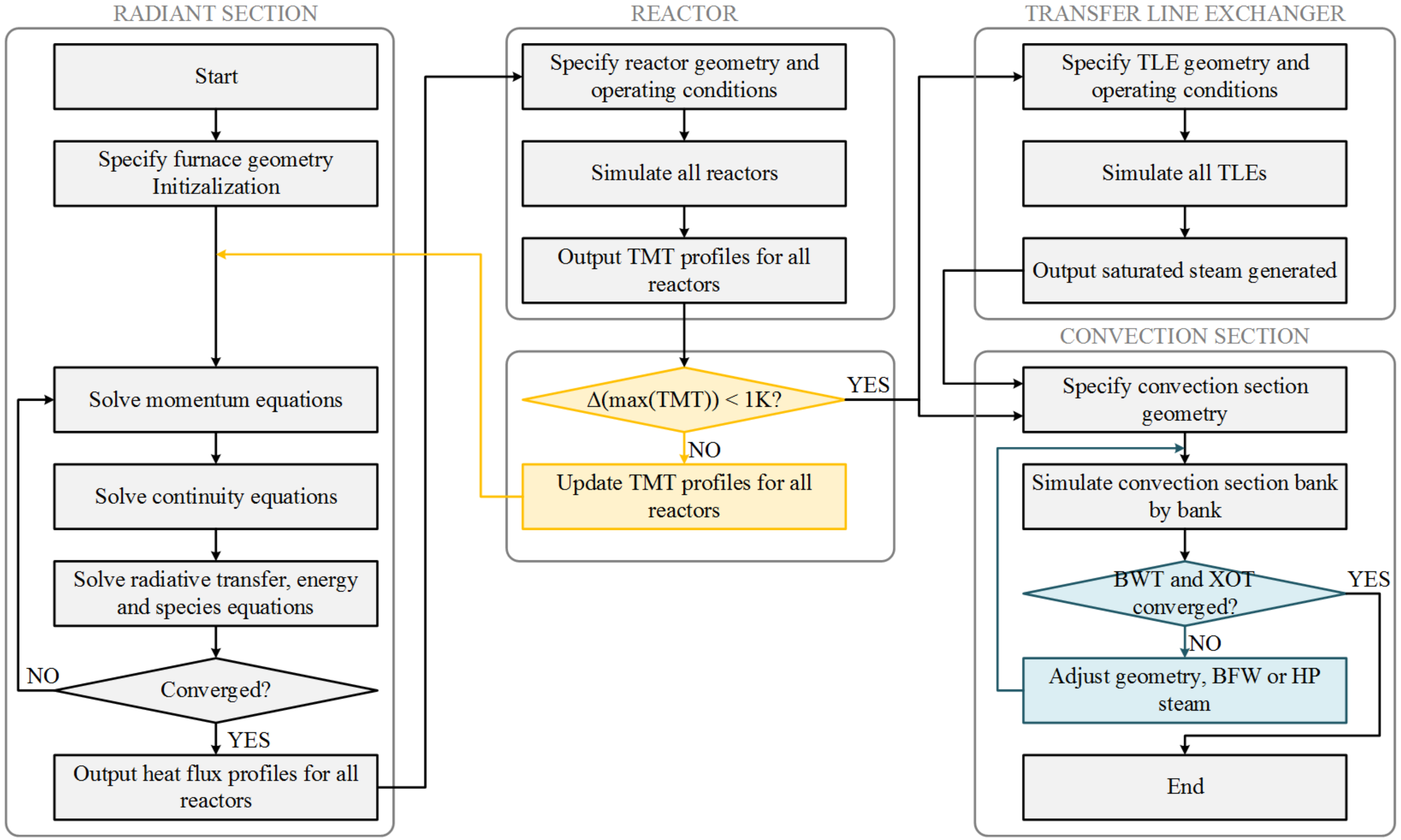
Simulation procedure: low emissivity case

Compare high vs low emissivity coil coating





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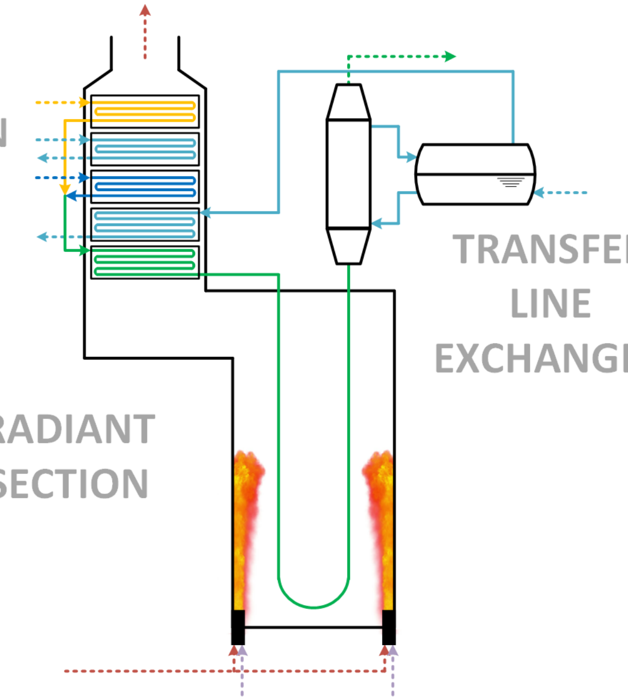
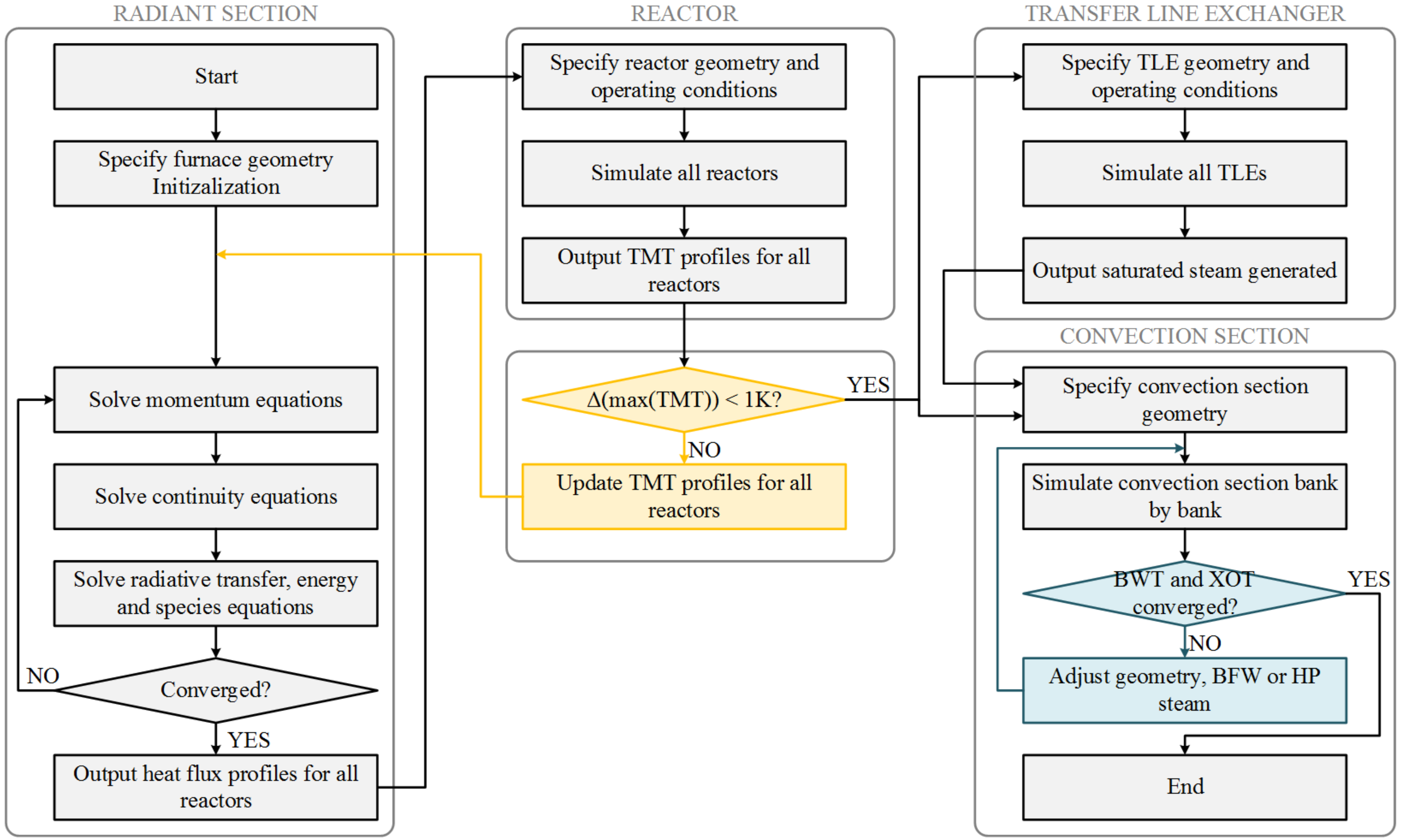
Simulation procedure: high emissivity case

Higher coil emissivity → more energy to process gas → over cracking





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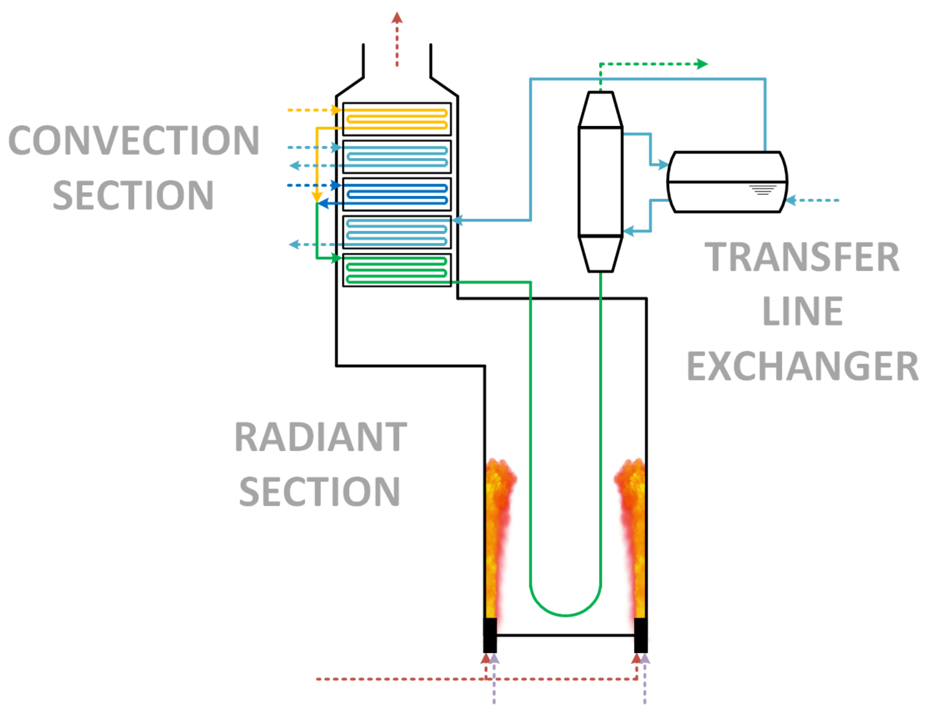
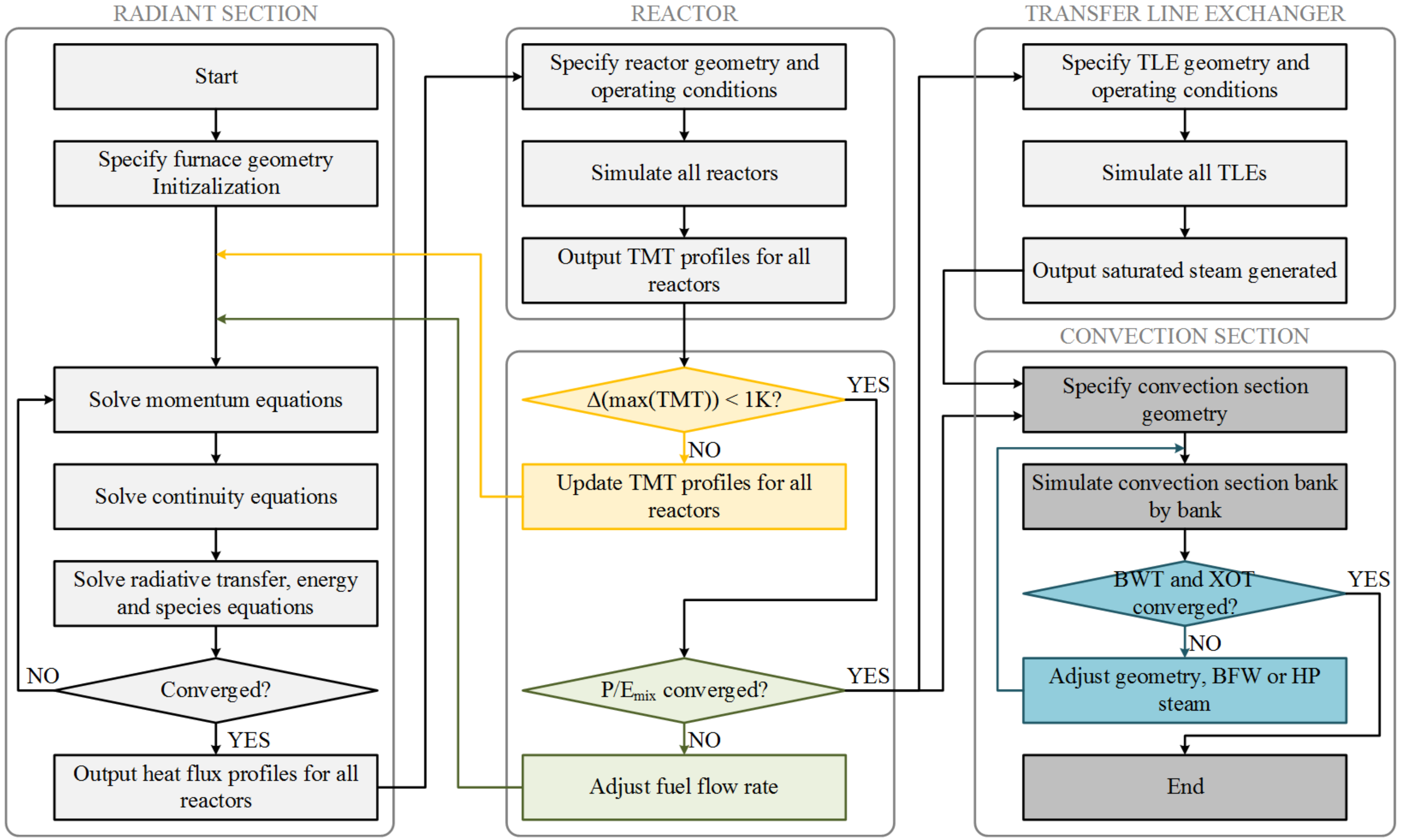
Simulation procedure: high emissivity case

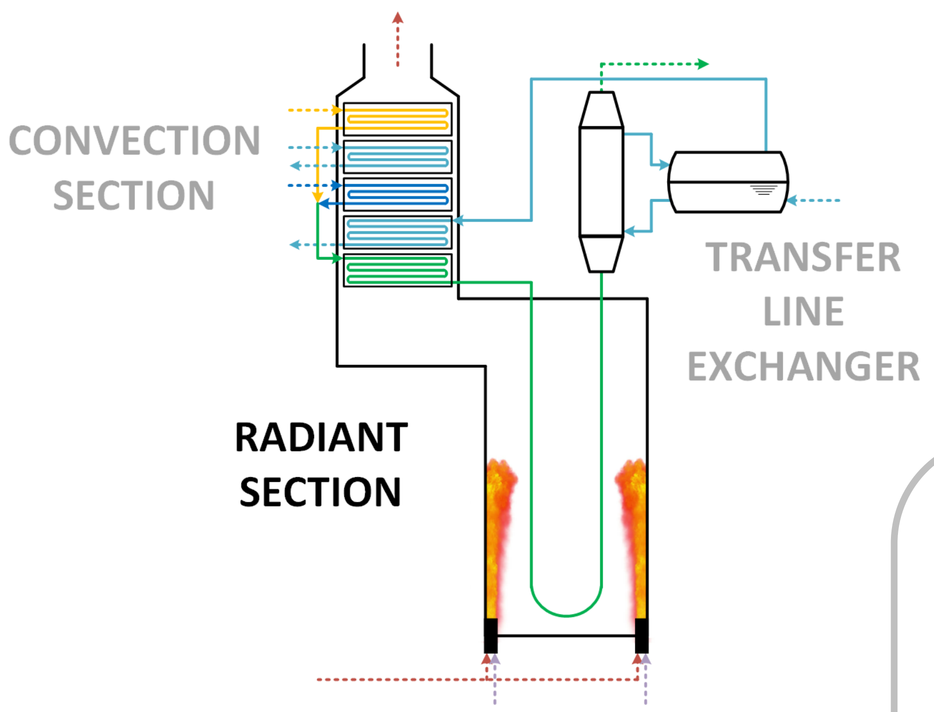
Higher coil emissivity → more energy to process gas → over cracking → reduce fuel





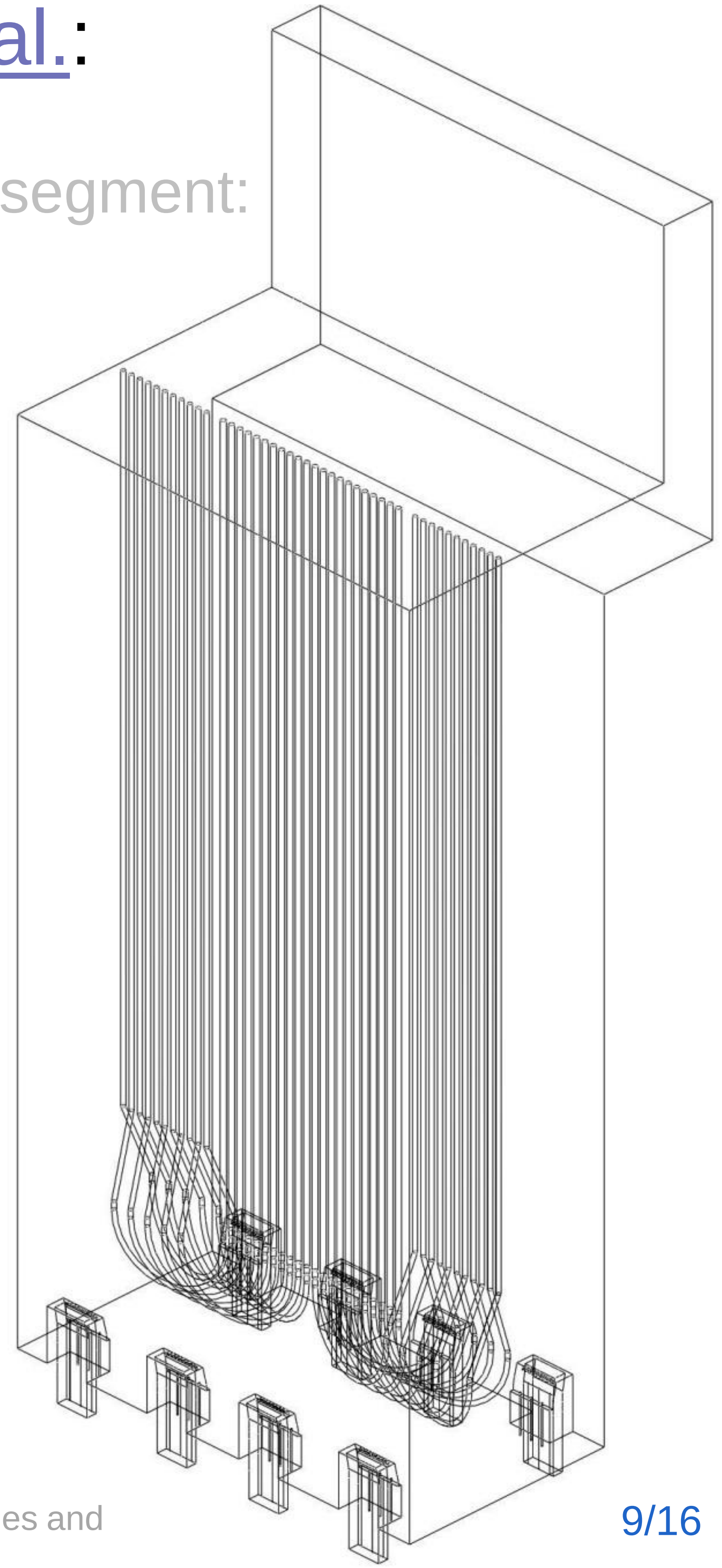
Geometry & operating conditions

Ultra Selective Conversion (USC) furnace simulated by Zhang et al.:



- 100 % floor fired
- U-coil reactor
- 22 reactor coils
- Naphtha feedstock

Simulated furnace segment:



Numerical models – CFD and COILSIM1D

- RANS k-ε turbulence modelling
- Discrete ordinates radiation using an exponential wide band model
- Two-step combustion model
- TMT coupling with COILSIM1D

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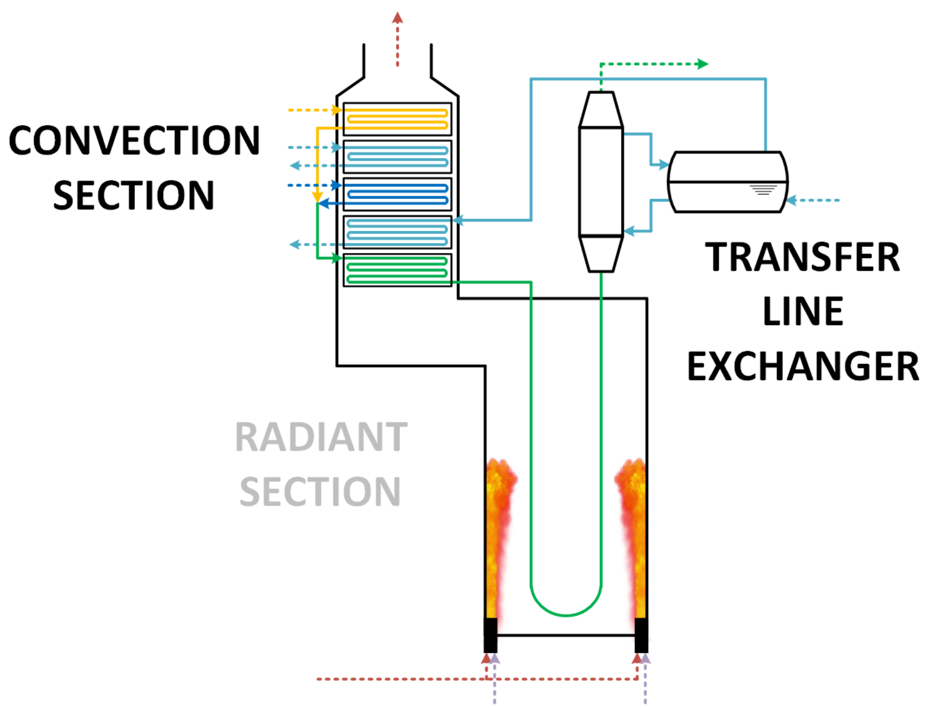
Zhang, Yu, Schietekat, C., Qian, F., Van Geem, K., & Marin, G. (2015). Impact of flue gas radiative properties and burner geometry in furnace simulations. *AICHE JOURNAL*.

Geometry & operating conditions

Convection section as simulated by Verhees et al.:



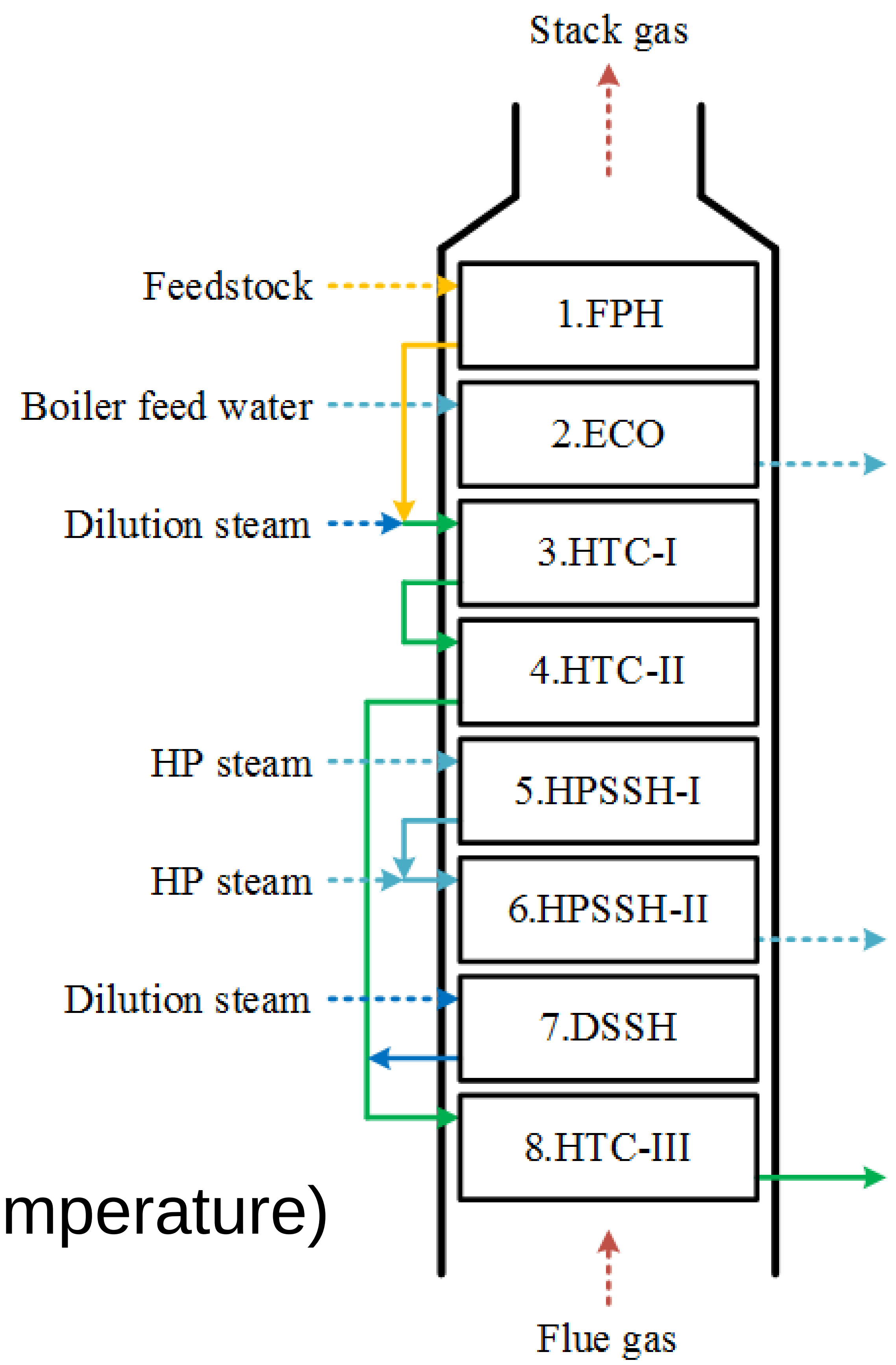
Numerical models – CONVEC-1D

1D heat transfer simulation tool
Process gas side:

- Two phase boiling models

Flue gas side:

- Convective flow over horizontal bank



Transfer line exchanger: ultraselective quench cooler

Double pipe exchanger combining two coils (770 K outlet temperature)

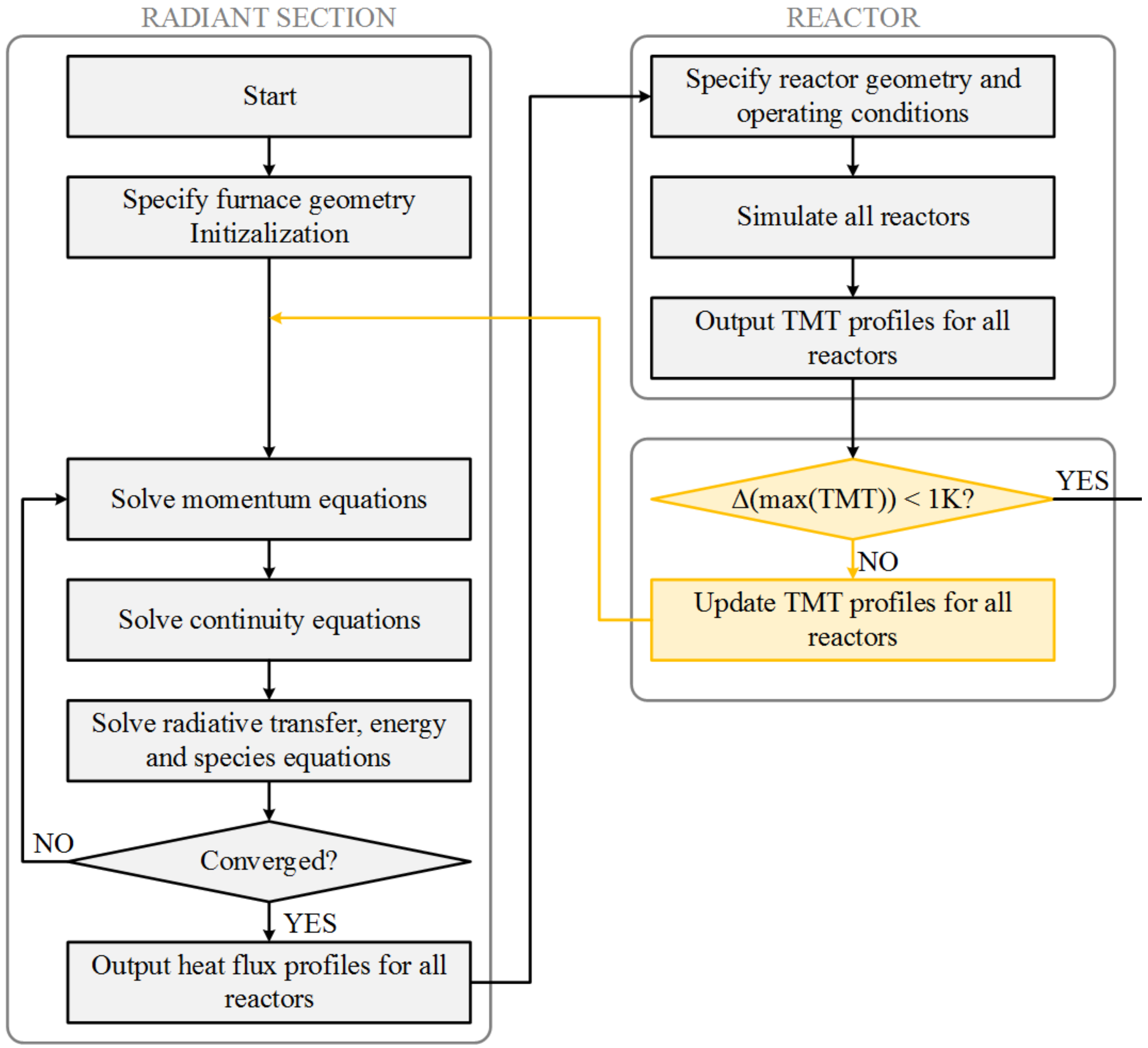
Verhees, P., Amghizar, I., Goemare, J., Akhras, A. R., Marin, G., Van Geem, K., & Heynderickx, G. (2016). 1D model for coupled simulation of steam cracker convection section with improved evaporation model. *CHEMIE INGENIEUR TECHNIK*.

Simulation results: low emissivity case

Simulation results radiant section

Radiant section	
Total fuel flow rate [kg/s]	1.1108
Flue gas bridge wall temperature [K]	1370
Percent of total heat flux via radiation [%]	77.88

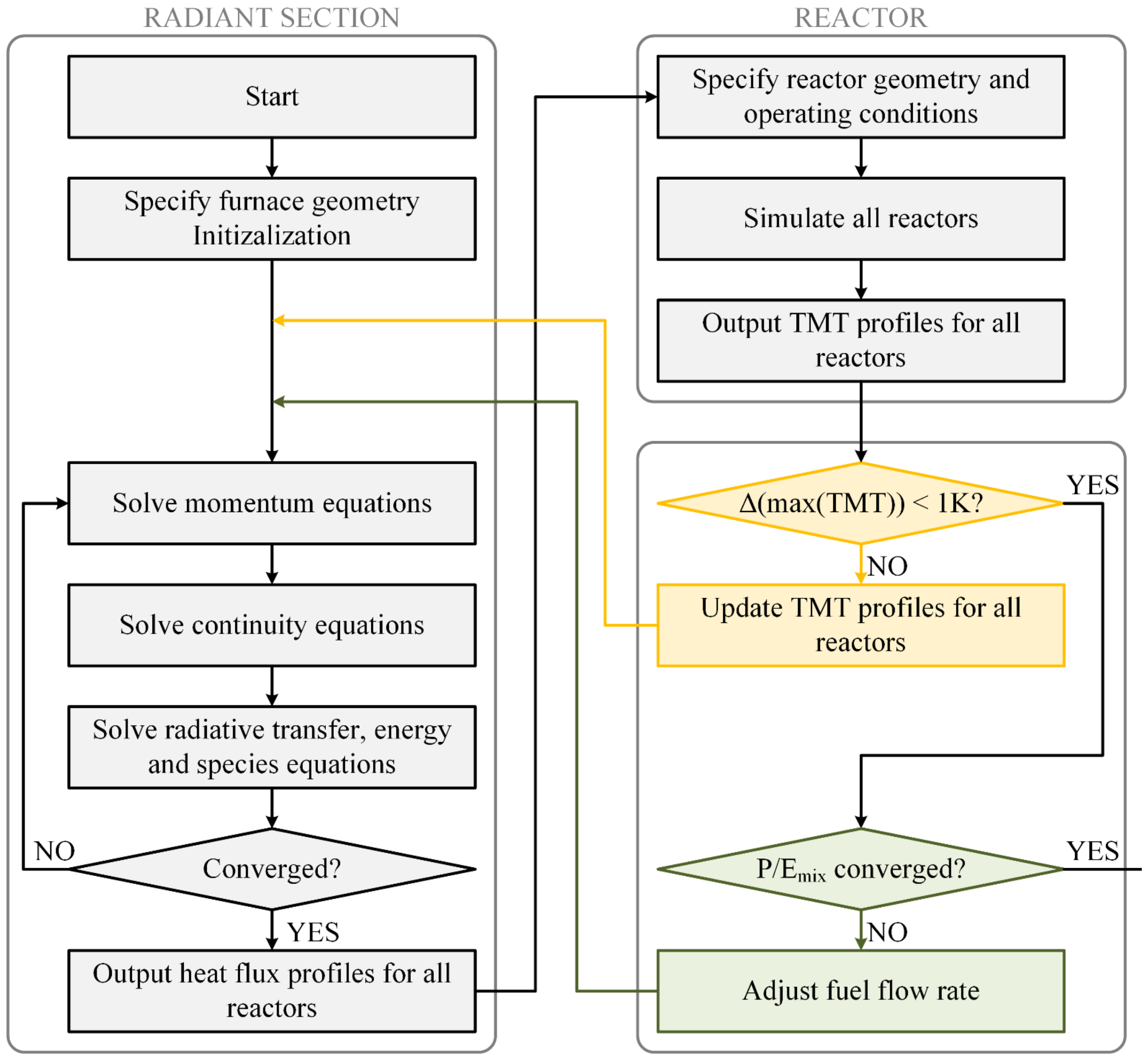
Reactor	
Mixing-cup average COT [K]	1146.1
Average ethene yield [wt%]	28.89
Average propene yield [wt%]	15.25
Mixing-cup average P/E	0.5284



Simulation results: low vs high emissivity case

Simulation results radiant section

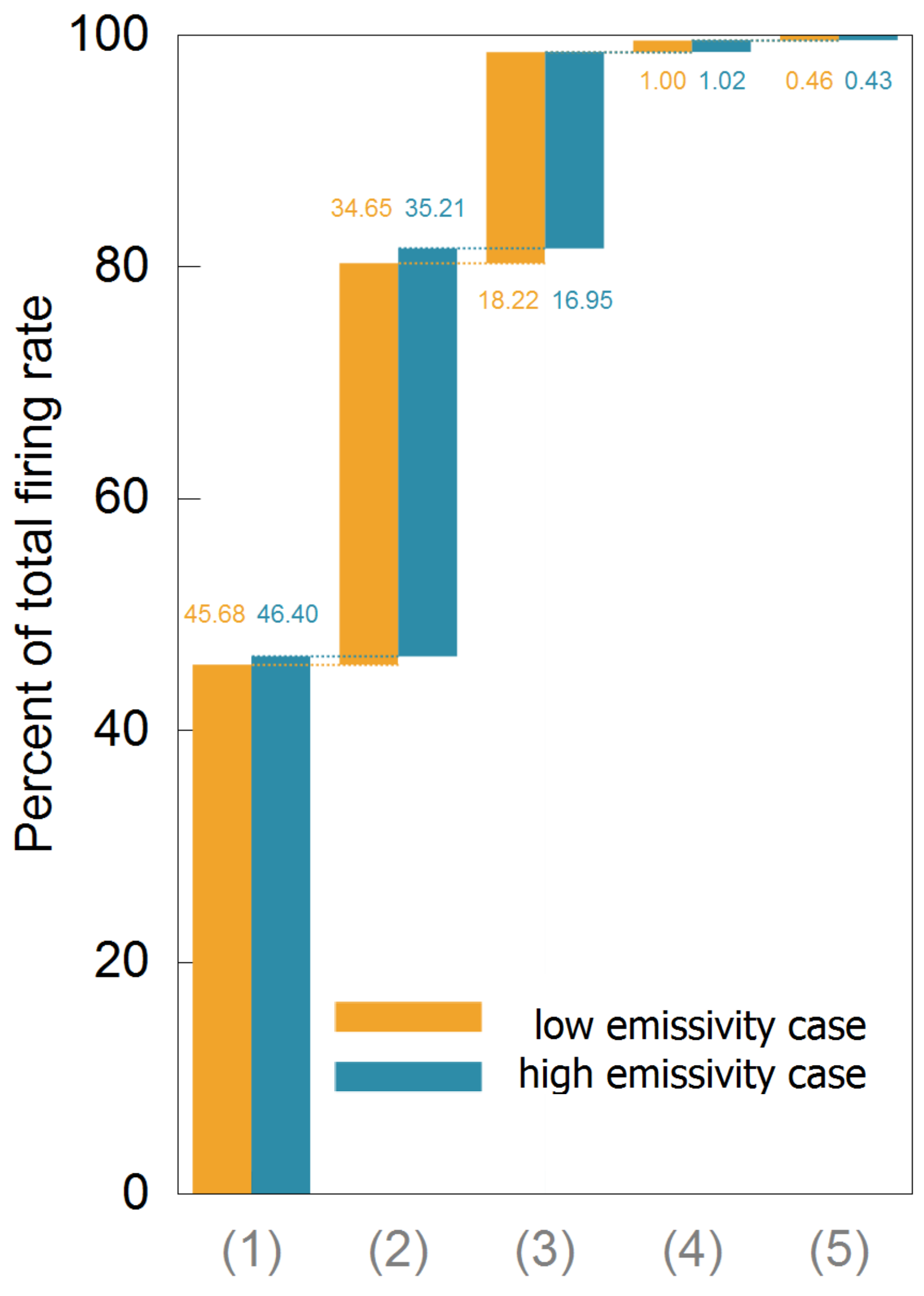
Radiant section	low emissivity	high emissivity
Total fuel flow rate [kg/s]	1.1108	1.0916 ↓
Flue gas bridge wall temperature [K]	1370	1356 ↓
Percent of total heat flux via radiation [%]	77.88	79.33 ↑
Reactor		
Mixing-cup average COT [K]	1146.1	1145.3
Average ethene yield [wt%]	28.89	28.88
Average propene yield [wt%]	15.25	15.25
Mixing-cup average P/E	0.5284	0.5284



Overall energy balance

After performing convection section and transfer line exchanger simulations

		low emissivity	high emissivity	
	Total fired duty [kW]	56628	55652	↓
(1)	Total reactor duty [kW]	25868	25820	~
(2)	Total preheating duty convection section [kW]	19620	19593	~
(3)	Total energy recovery duty convection section [kW]	10316	9435	↓
(4)	Total losses from radiant section [kW]	566	566	~
(5)	Total losses through stack [kW]	259	238	↓
	Furnace efficiency radiant section [%]	45.68	46.40	↑



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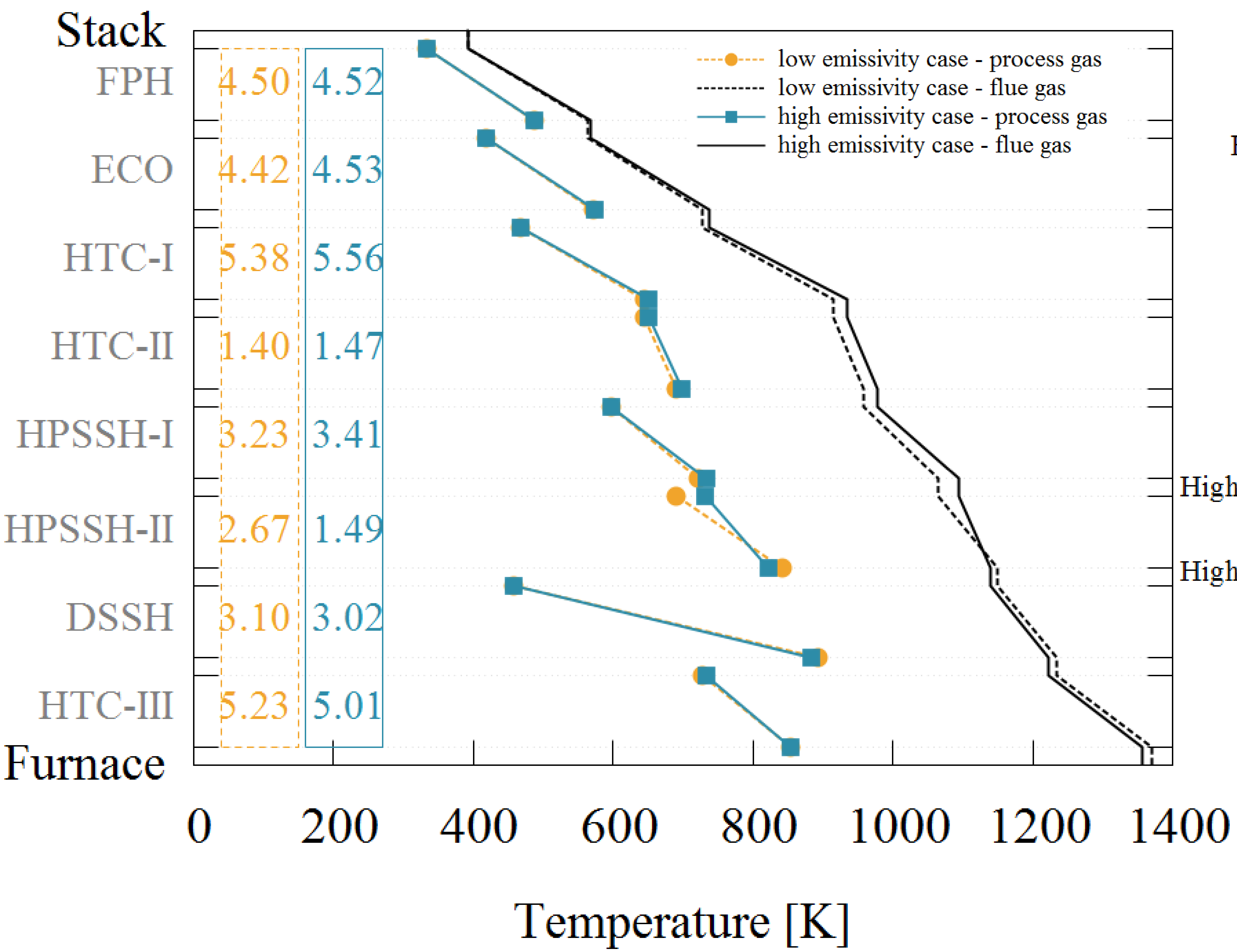
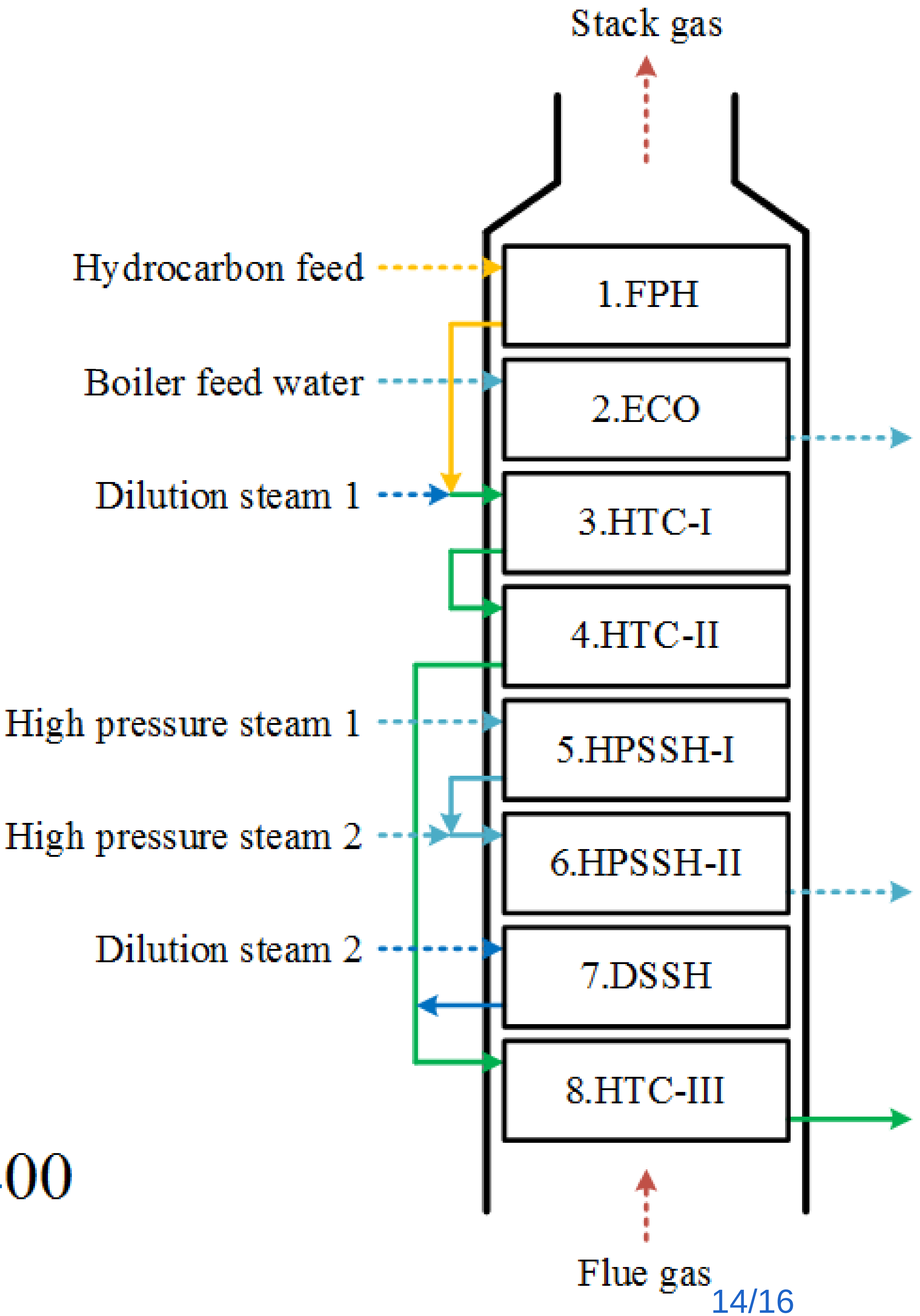
Closer look at the energy balance



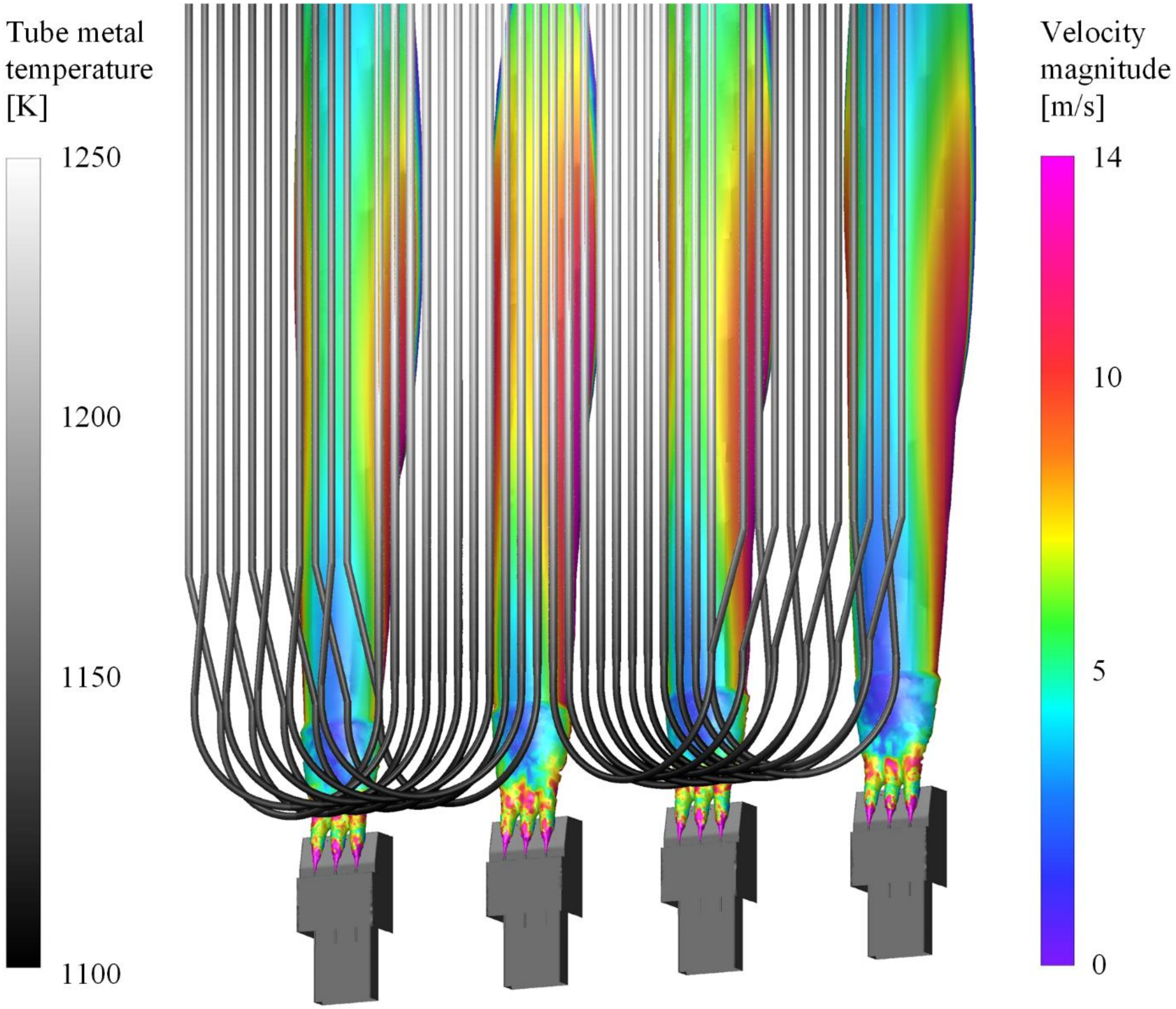


Conclusions

Increasing the coil emissivity results in:

- Increased energy efficiency of the radiant section by 0.70 % absolute
- Reduced firing rate by 1.73 %
- Reduced bridge wall temperature of 14 K

→ minor operating changes to convection section required



Reyniers, P., Vangaever, S., Visser, C., Jakobi, D., Heynderickx, G., Marin, G. & Van Veem, K. (2018). Computational Fluid Dynamics-Based Study of a High Emissivity Coil Coating in an Industrial Steam Crackier. *Industrial & Engineering Chemistry Research. (submitted)*

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