INTERREG FWVL GUEST LECTURES, ONLINE, APRIL 28, 2026

Catalytic Reaction and Reactor Engineering for Bio-Gas Valorization

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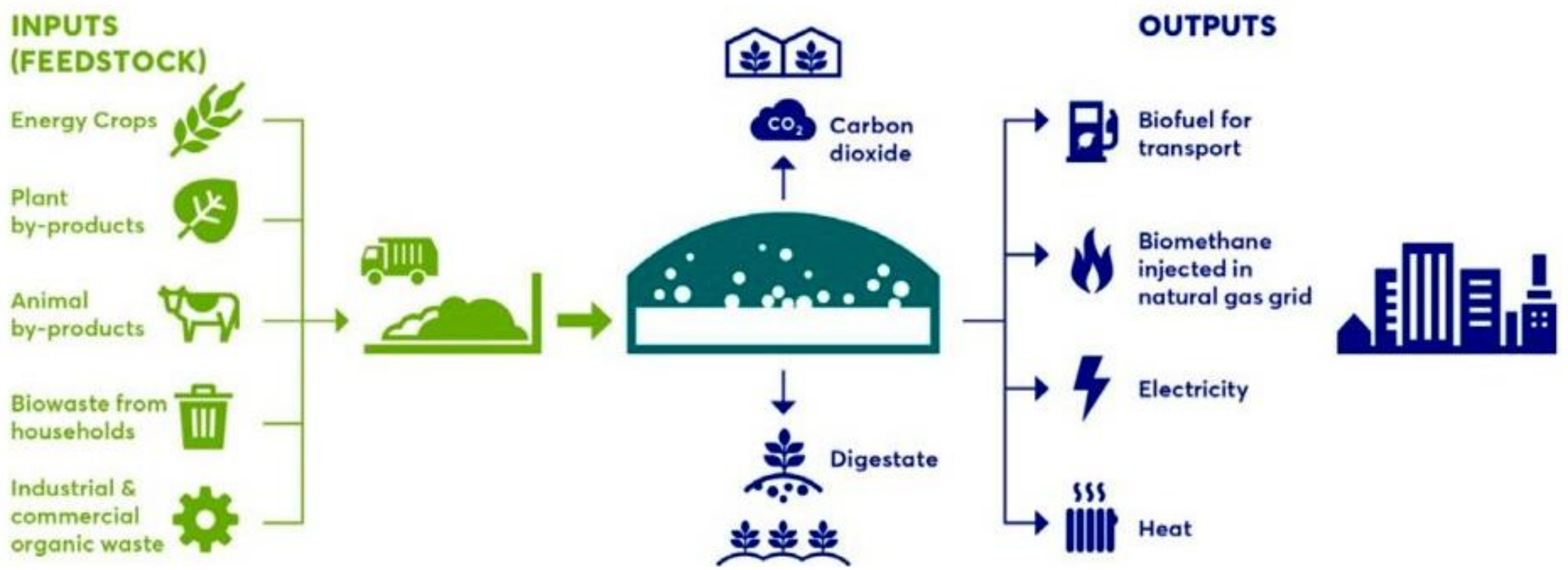
biogas

biogas = CH_4 (biomethane, ~50-70%) **+ CO_2** (~24-45%)



what if we could to transform it into chemicals?

biogas to chemicals

- reactions
  - CH_4
    - steam reforming
    - pyrolysis
    - oxidative coupling
  - CO_2
    - dry reforming (with CH_4)
    - hydrogenation
    - reverse Boudouard
- reactors
  - exothermicity
    - multitubular
    - fluidized bed
  - endothermicity
    - fired furnaces
    - electrification

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outline

- introduction
- catalytic reaction engineering
  - hydrogen production/methane pyrolysis
  - gas phase vs surface reactions/catalyst descriptors
- catalytic reactor engineering
  - electrification/EltectroThermal Fluidized Bed reactor (ETFB)
  - ETFB reactor model
- conclusions & perspectives

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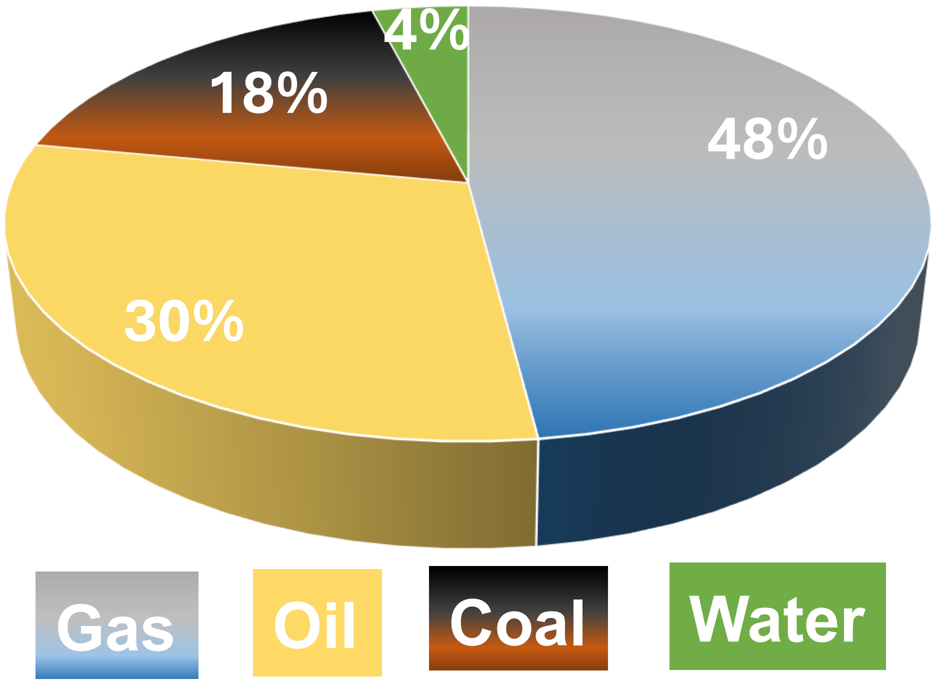
CH_4 conversion → H_2 production

H_2 production feedstocks



Technology	reaction	ΔH kJ/mol	cost ($/kg)	GWP (kg CO_2 eq)
Steam Methane Reforming	$CH_4 + H_2O \leftrightarrow CO + 3H_2$	206	2.08	11.9
SMR + CCS			2.27	3.7
Coal Gasification	$C + H_2O \leftrightarrow CO + H_2$	-130	1. 34	22.9
CG + CCS			1. 63	4.8
Electrolysis	$2H_2O \leftrightarrow 2H_2 + O_2$	285	>3	>0.7

Catalytic Methane Decomposition:

$$CH_4 \rightarrow C(s) + 2H_2(g) \qquad \Delta H = \mathbf{74}\ \text{kJ/mol}$$

CDM on carbonaceous catalyst:

- ❑ less energy-intensive
- ❑ Less greenhouse gas emission
- ❑ Produces H_2 with high purity
- ❑ Cheap catalyst
- ❑ Sulfur-resistive catalyst

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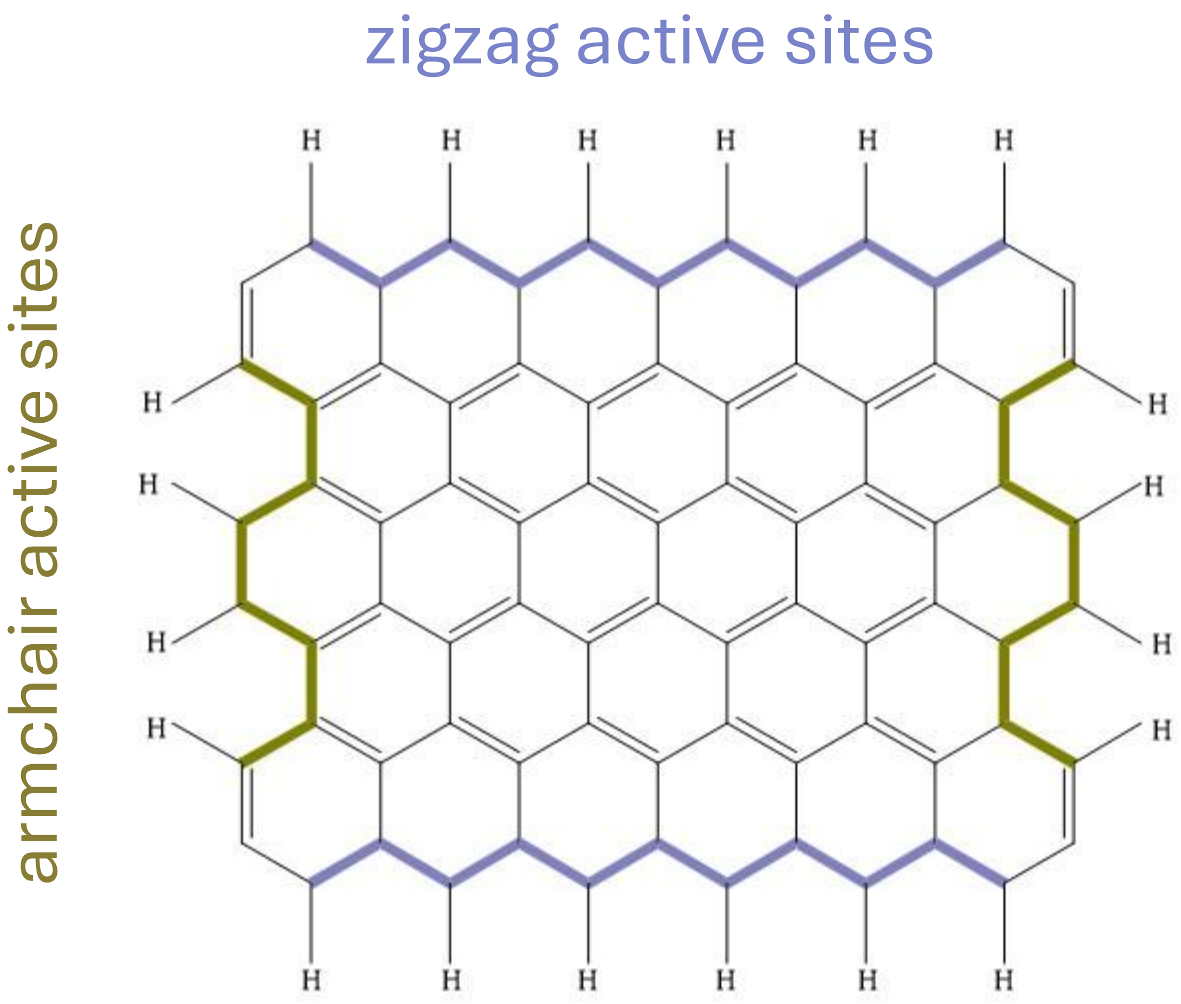
Gholami et al. J. Ind. Eng. Chem. 2026 153 240-278

CH_4 pyrolysis

- gas phase reactions
  - AramcoMech 3.0
- surface reactions
  - Lacroix:
    - 66 species
    - 275 reactions
  - catalyst descriptors
    - ordered vs amorphous



C(B), Ċ(S), Ċz(S), H(S), Hz(S)

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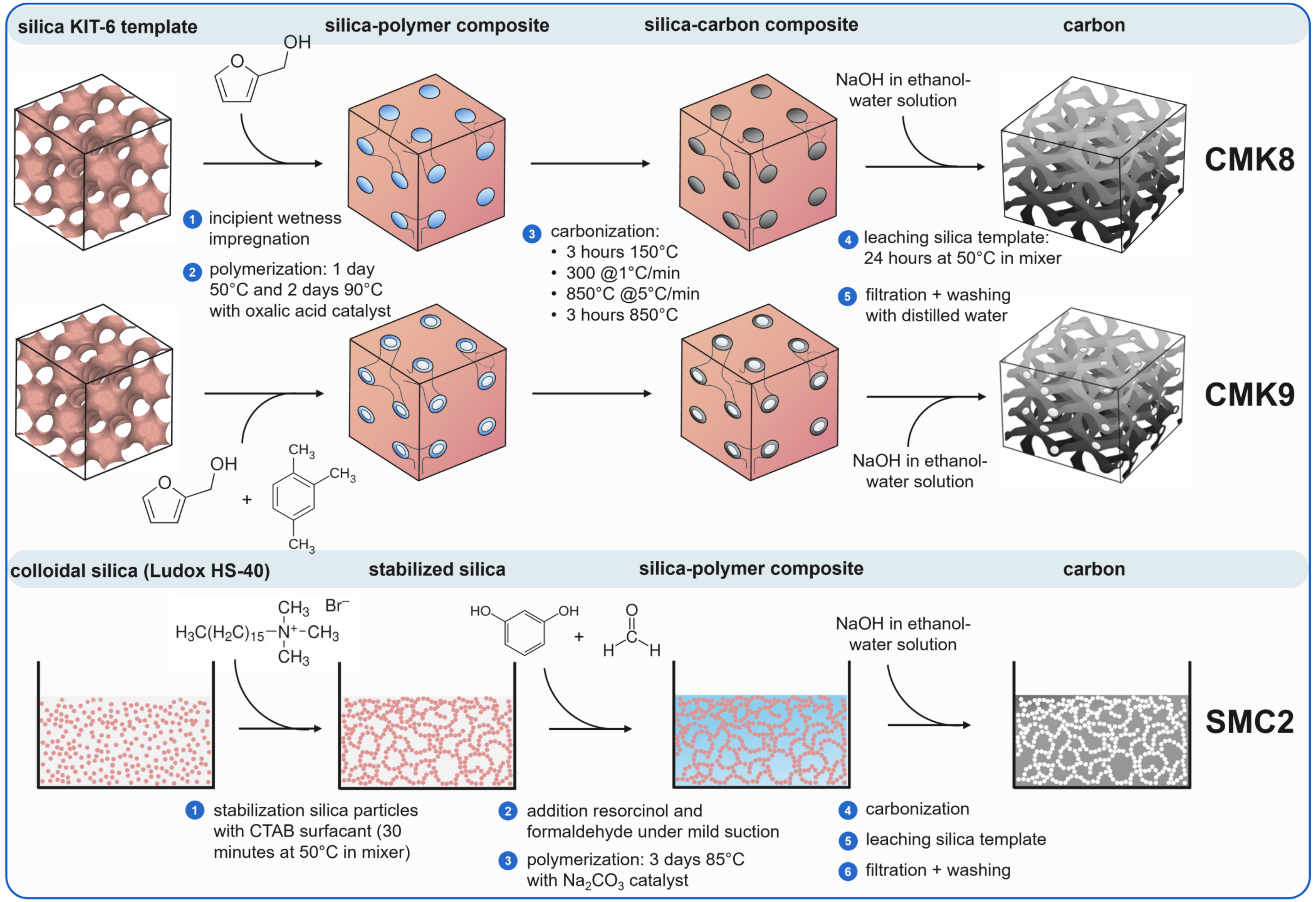
Zhou C.W. et al. Comb & Flame 2018 197 423-438
Lacroix et al. Carbon 2010 48 132-144

carbonaceous materials synthesis



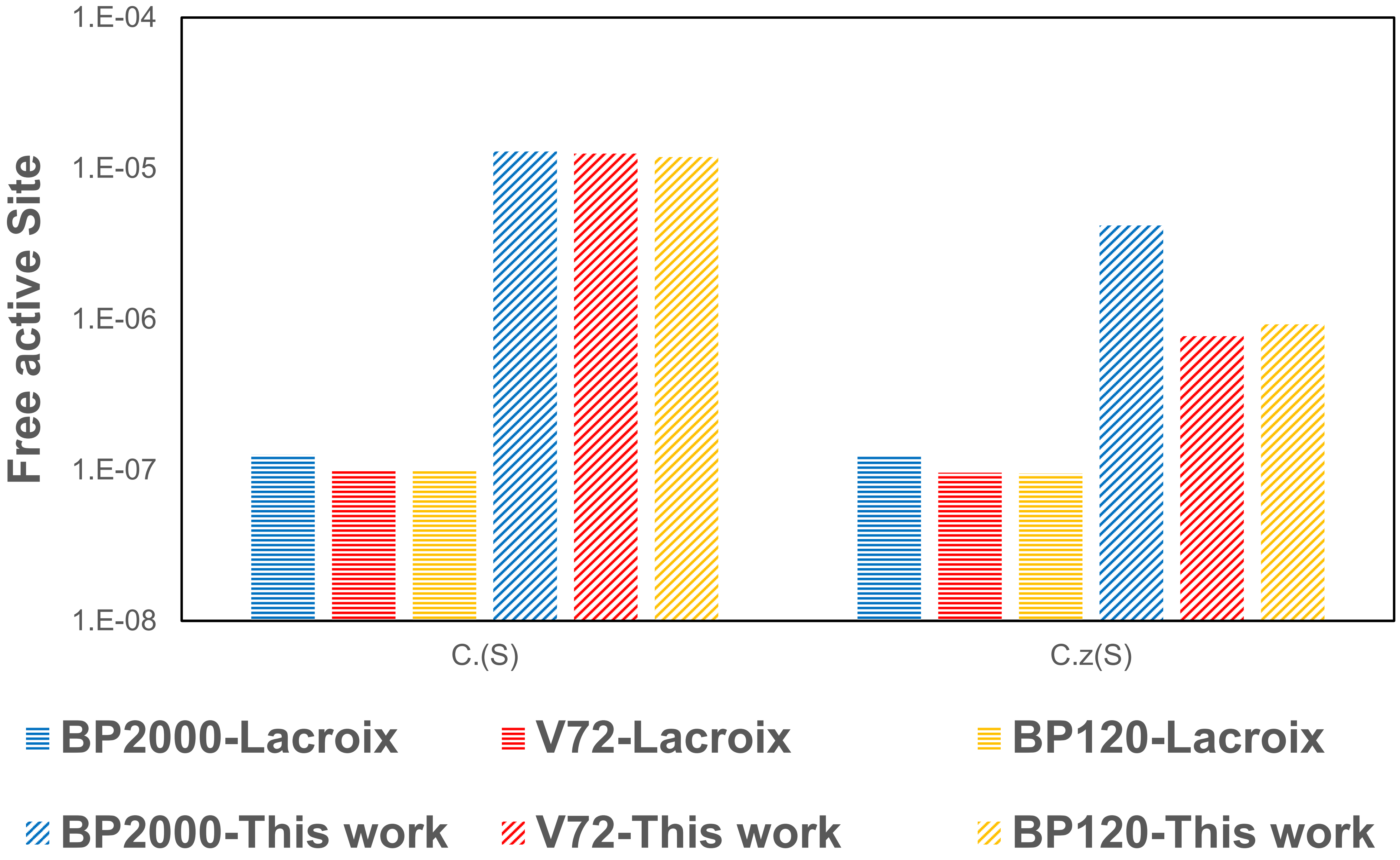
carbon black surface properties carbon black.			
	BP2000	V72	BP120
total number of active sites (g^{-1})	$2\ 10^{19}$	$1\ 10^{18}$	$7\ 10^{17}$
active site density ($\frac{mol}{cm^2}$)	$2.1\ 10^{-12}$	$7.3\ 10^{-13}$	$3.8\ 10^{-12}$
surface area (m^2/g)	1516	224	30.5

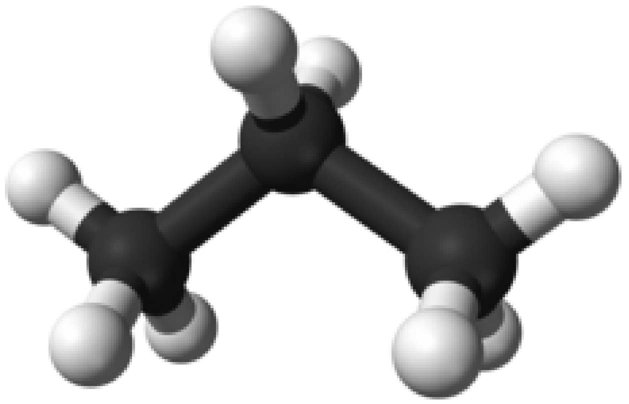
De Langhe et al. Ind. Eng. Chem. Res. 2025 64 6878-6896
Zareghorbaei et al. Ind. Eng. Chem. Res. 2025 64 20919-20929

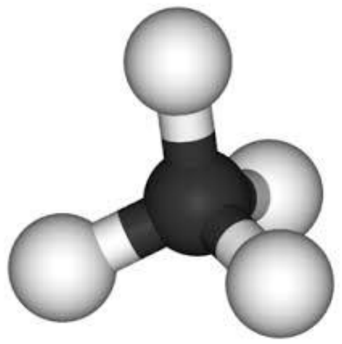
selected surface reactions

	surface reactions*	A_f	n_f (-)	Ea_f (kJ/mol)	A_r	n_r (-)	Ea_r (kJ/mol)
1.a	$C(B) + H(S) + \dot{H} \leftrightarrow \dot{C}(S) + H_2$	$5\ 10^{7}$	1.8	70.2	$1.4\ 10^{7}$	1.8	36.3
1.z	$C(B) + Hz(S) + \dot{H} \leftrightarrow \dot{C}z(S) + H_2$						
2.a	$C(B) + H(S) + C\dot{H}_3 \leftrightarrow \dot{C}(S) + CH_4$	$6.6\ 10^{11}$	0	62.7	$1.4\ 10^{12}$	0	30.5
2.z	$C(B) + Hz(S) + C\dot{H}_3 \leftrightarrow \dot{C}z(S) + CH_4$						
3	$C(B) + H(S) + C_2\dot{H}_5 \leftrightarrow \dot{C}(S) + C_2H_6$	$1\ 10^{11}$	0	62.7	$5\ 10^{11}$	0	10.8
4	$C(B) + H(S) + C_2\dot{H}_3 \leftrightarrow \dot{C}(S) + C_2H_4$	$1\ 10^{11}$	0	54.3	$4.7\ 10^{11}$	0	40.9
5.a	$C(B) + H(S) \leftrightarrow \dot{C}(S) + \dot{H}$	$1.7\ 10^{16}$	0	470	$1\ 10^{14}$	0	0
5.z	$C(B) + Hz(S) \leftrightarrow \dot{C}z(S) + \dot{H}$						
5.a**	$C(B) + H(S) \leftrightarrow \dot{C}(S) + \dot{H}$	$6.7\ 10^{15}$	0	337.3	$1\ 10^{14}$	0	0
5.z*	$C(B) + Hz(S) \leftrightarrow \dot{C}z(S) + \dot{H}$	$1\ 10^{15}$	0	382	$1\ 10^{14}$	0	0

relevance surface reactions (C_3H_8 vs CH_4)



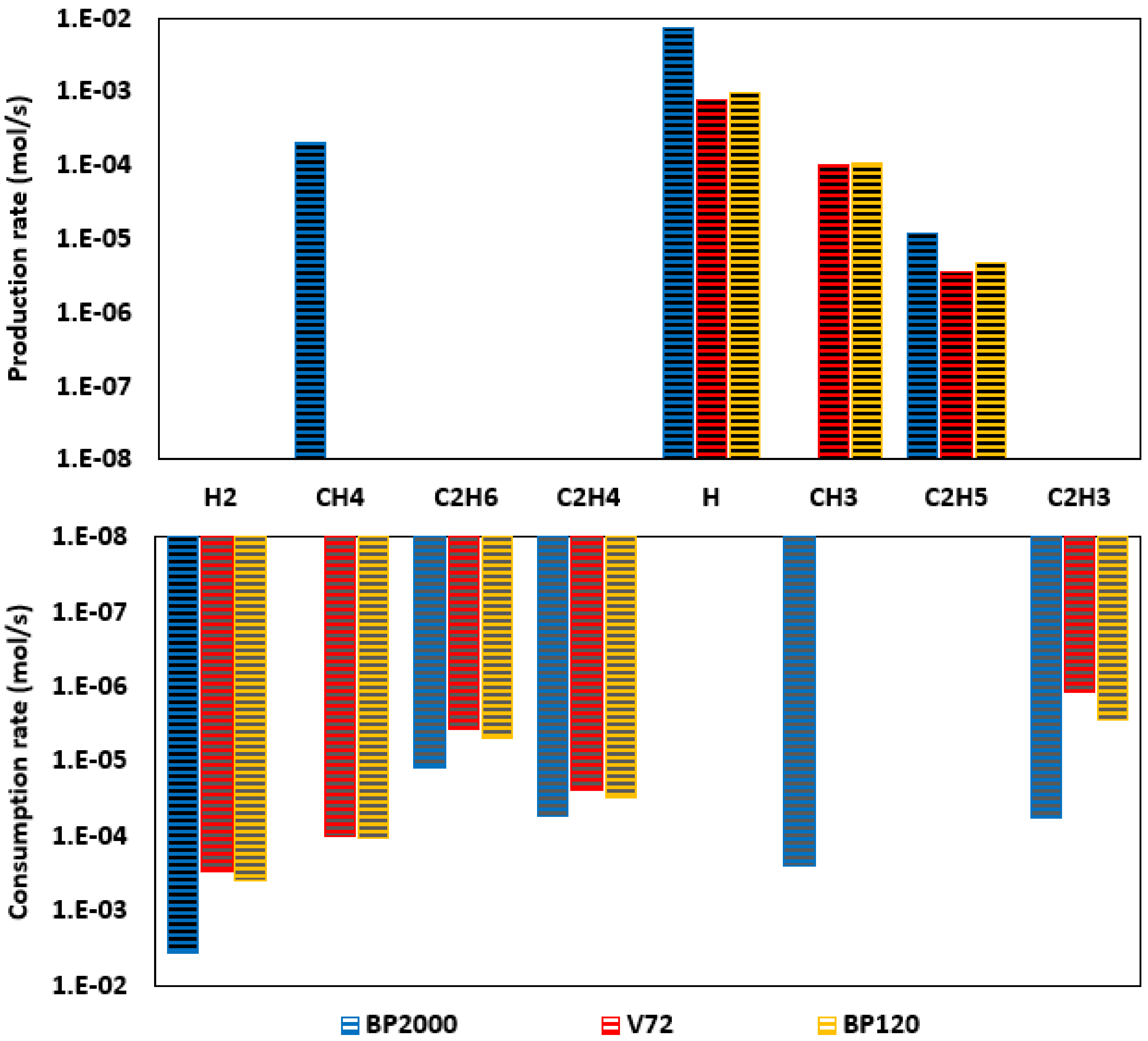




Lacroix et al. Carbon 2010 48 132-144
Zareghorbaei et al. Ind. Eng. Chem. Res. 2025 64 20919-20929

surface rates

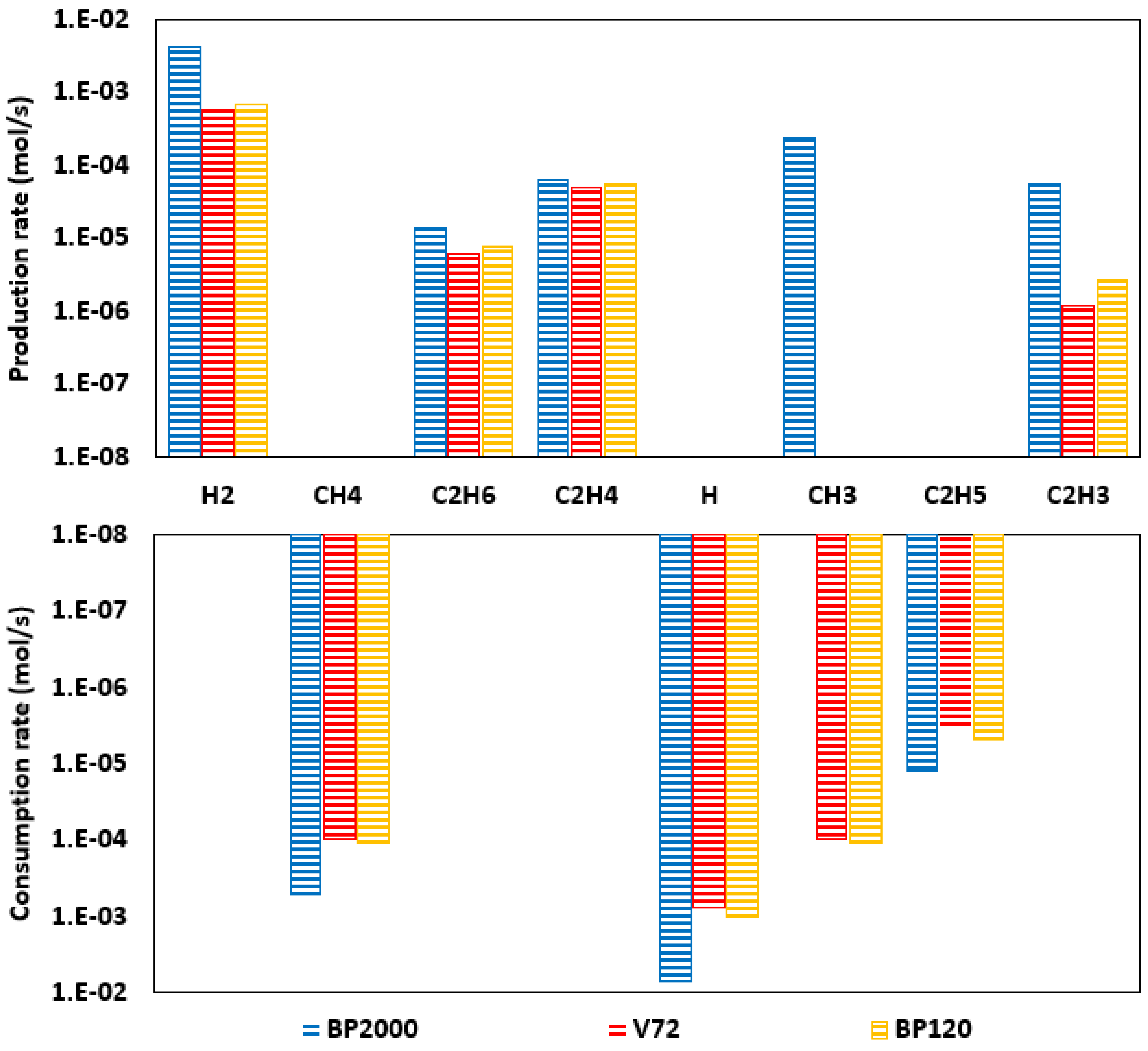
- H radical production
- methyl radical:
  - consumption (large surface area)
  - production (low surface area)
- methane: reverse of methyl radical



Zareghorbaei et al. Ind. Eng. Chem. Res. 2025 64 20919-20929

gas phase rates

- H radical reacts with CH_4 into H_2 and methyl radical
- methyl radical:
  - production (large surface area)
  - consumption (low surface area)
- methane: consumption only



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reaction pathway analysis

	surface reactions*
1.a	$C(B) + H(S) + \dot{H} \leftrightarrow \dot{C}(S) + H_2$
1.z	$C(B) + Hz(S) + \dot{H} \leftrightarrow \dot{C}z(S) + H_2$
2.a	$C(B) + H(S) + C\dot{H}_3 \leftrightarrow \dot{C}(S) + CH_4$
2.z	$C(B) + Hz(S) + C\dot{H}_3 \leftrightarrow \dot{C}z(S) + CH_4$
3	$C(B) + H(S) + C_2\dot{H}_5 \leftrightarrow \dot{C}(S) + C_2H_6$
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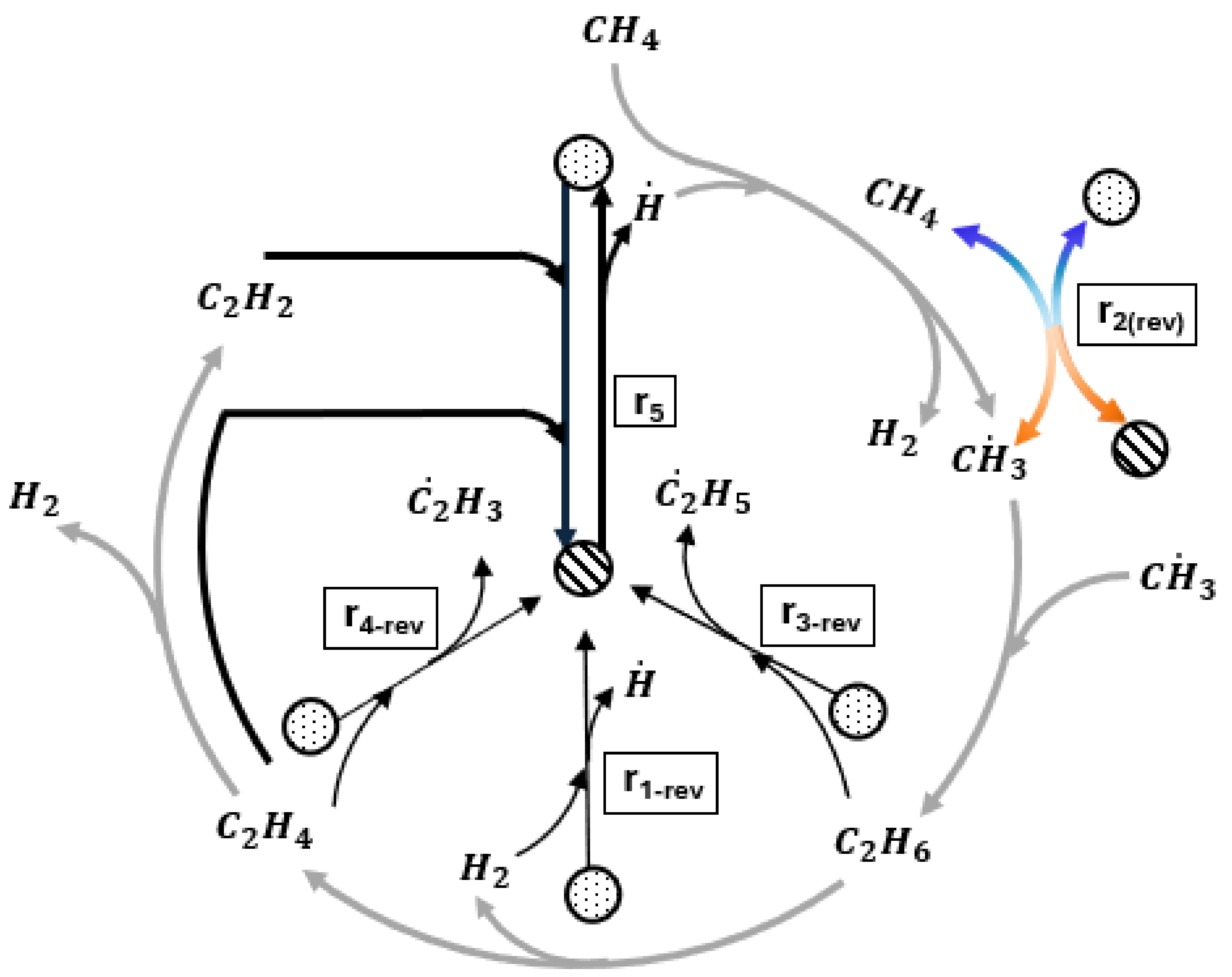
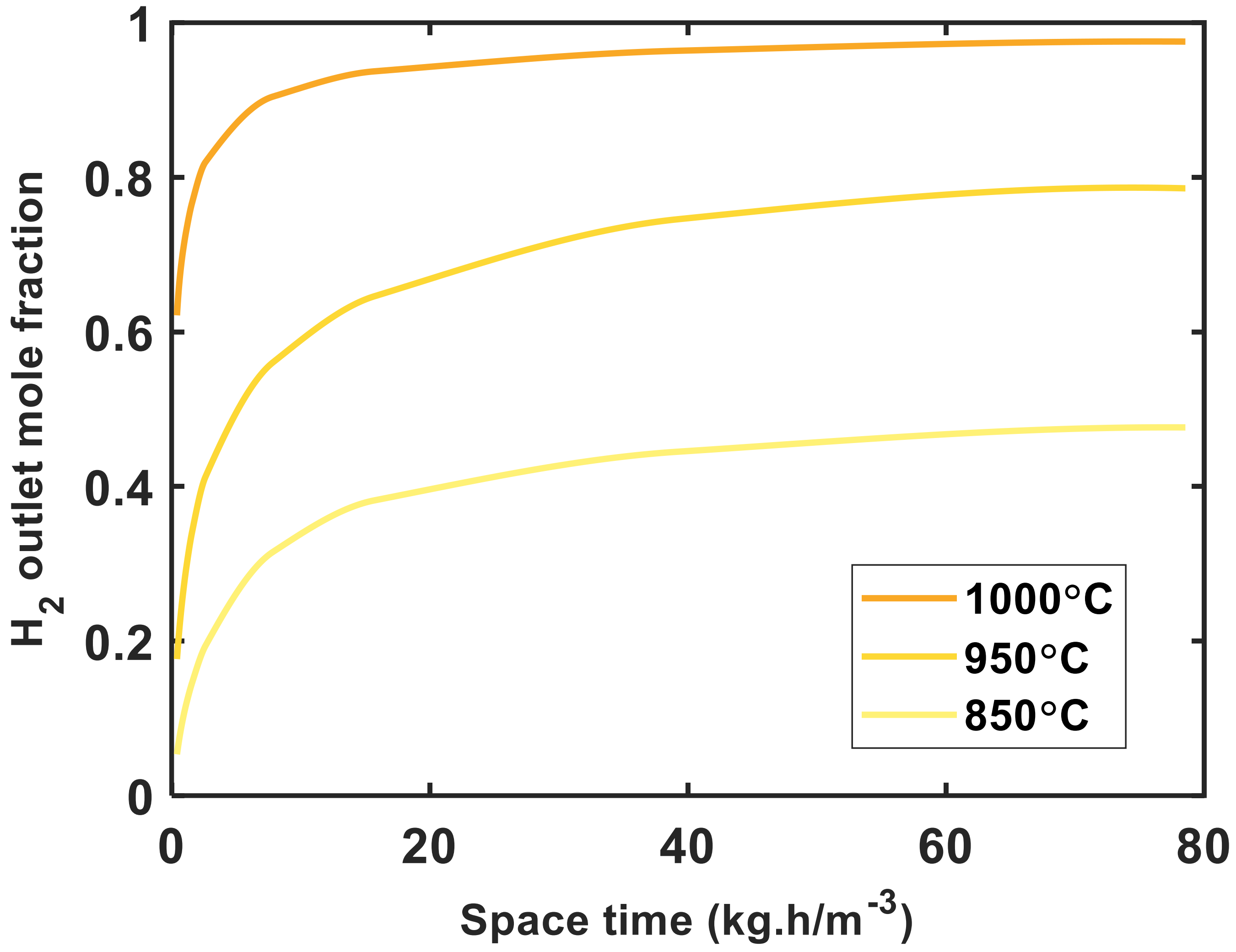
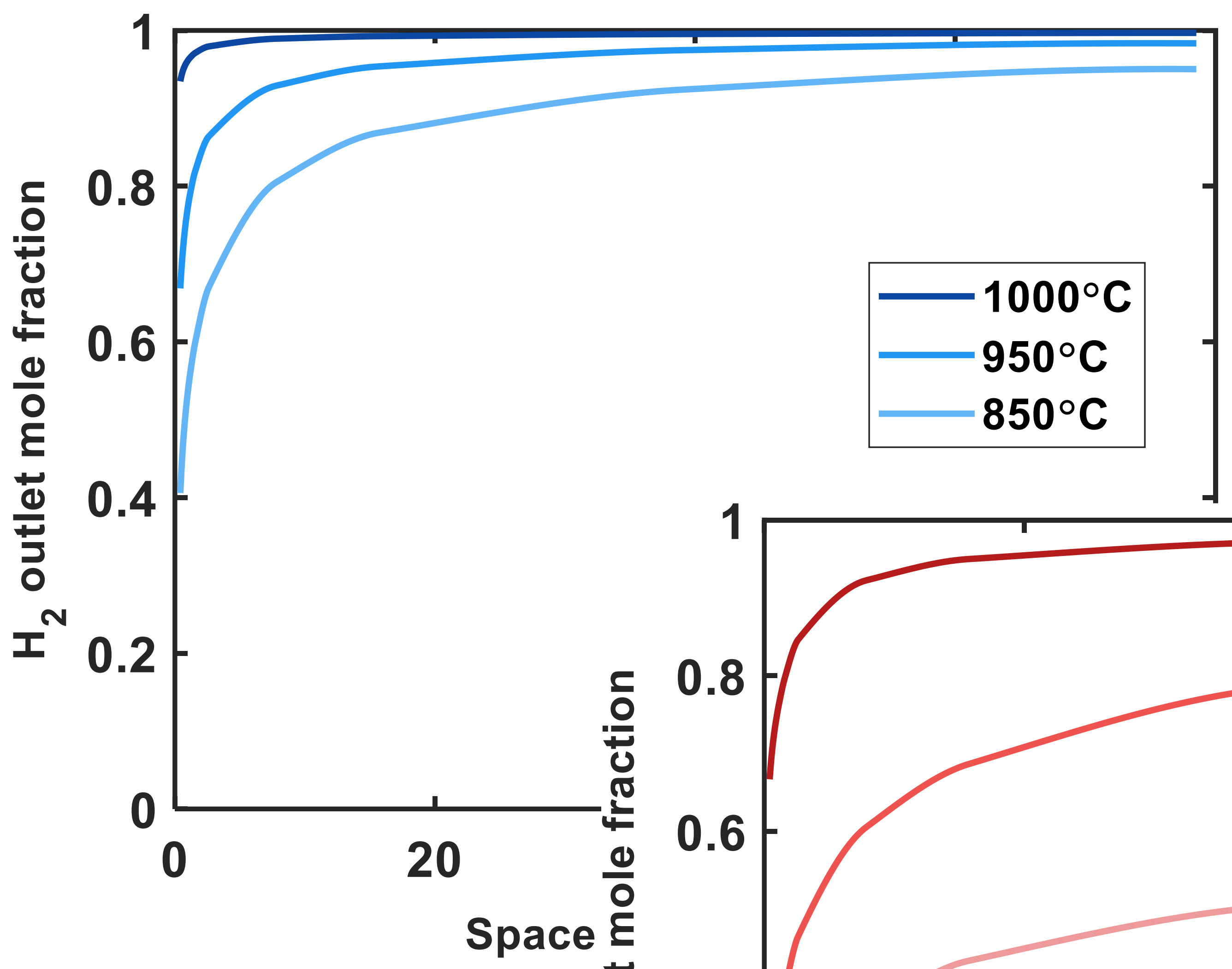
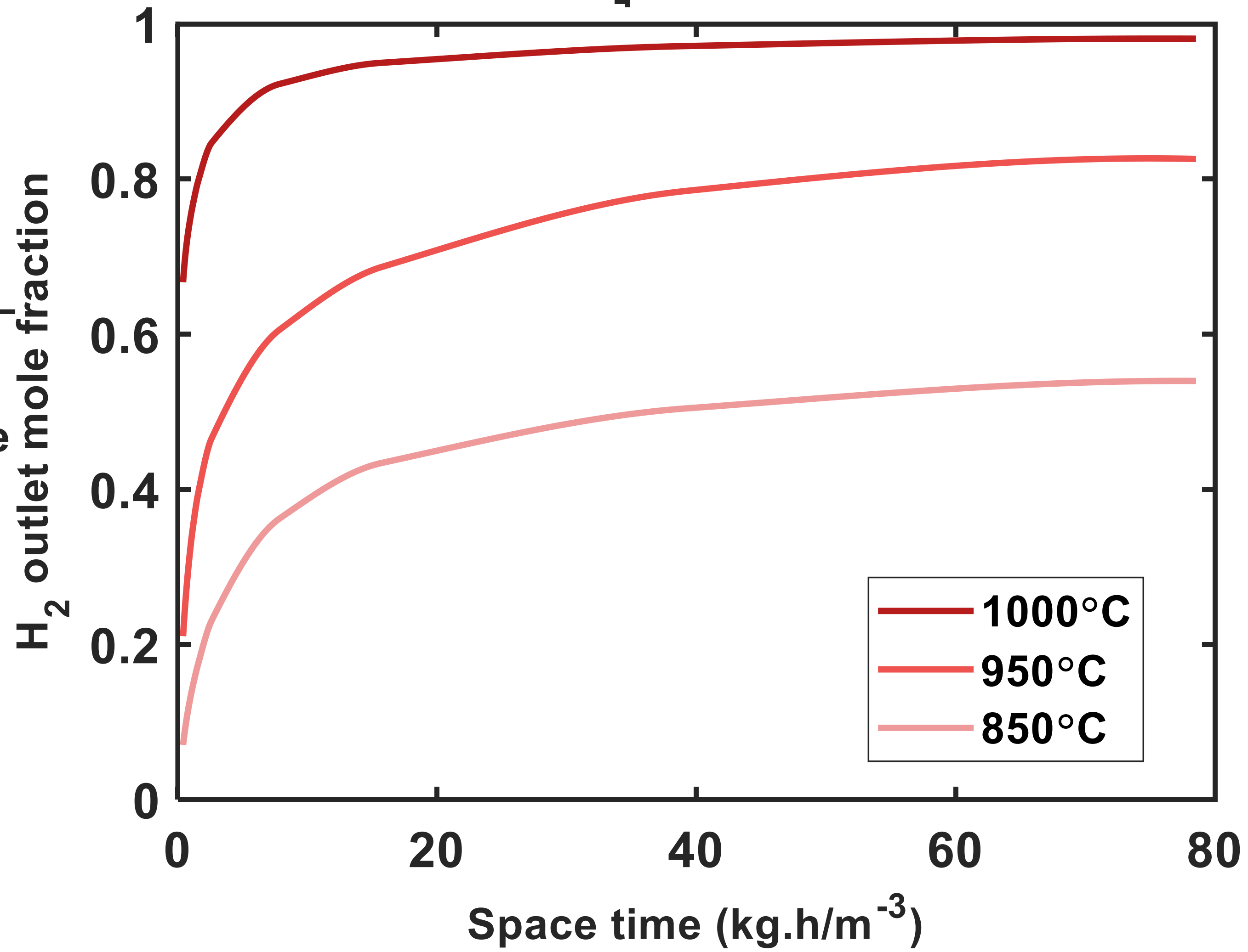


Zareghorbaei et al. Ind. Eng. Chem. Res. 2025 64 20919-20929

H_2 production over carbon catalysts







Zareghorbaei et al. Ind. Eng. Chem. Res. 2025 64 20919-20929

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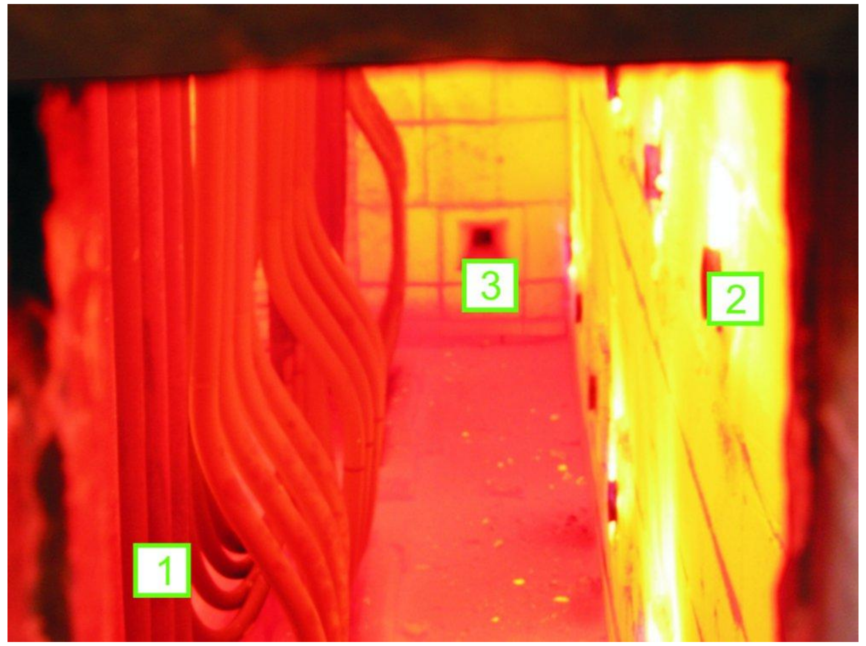
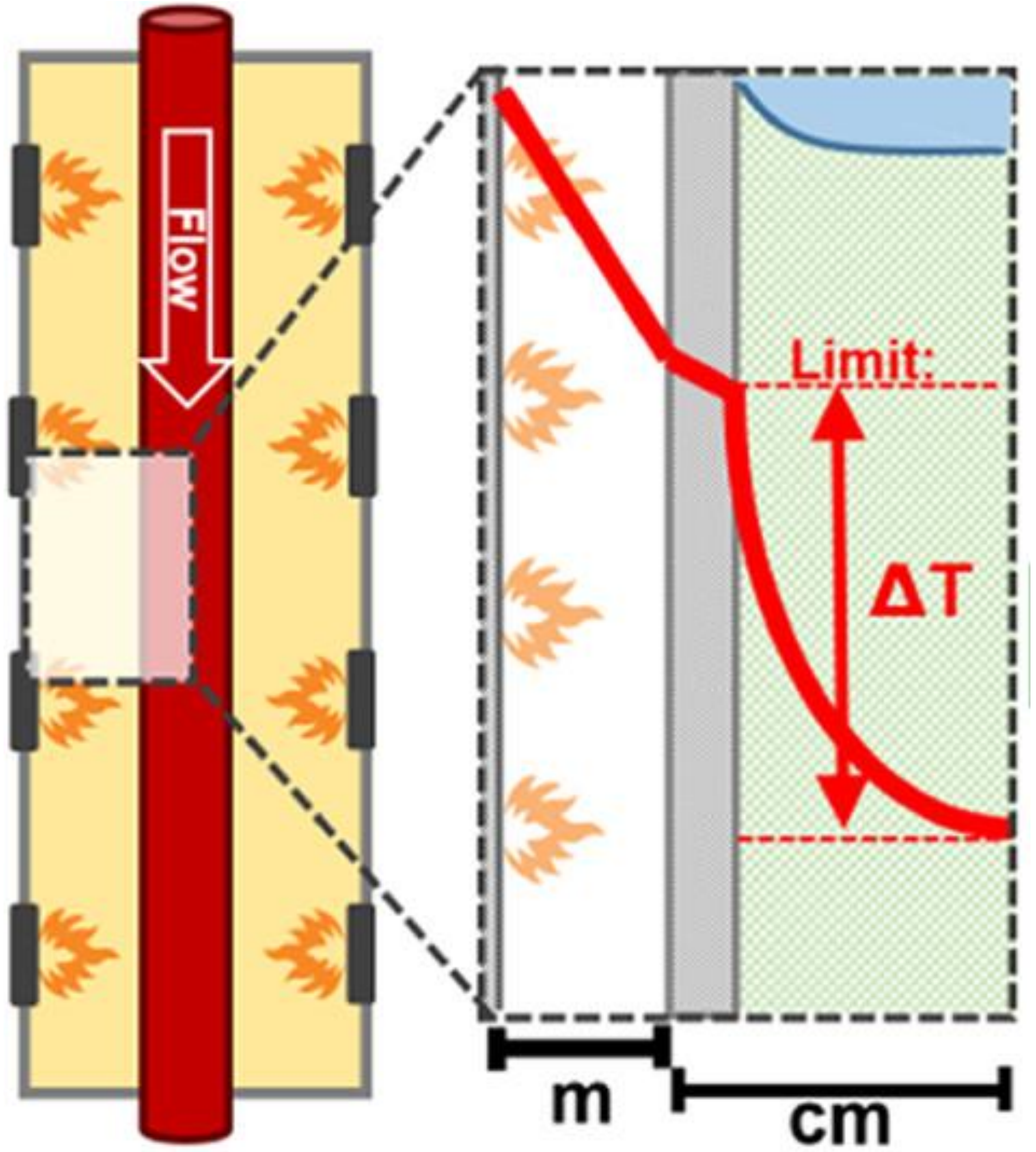
(strongly) endothermic reactions

– heat transport focused reactor design
  – narrow tubes
  – fired furnace
– pronounced temperature gradients





Wismann, et al. Ind. Eng. Chem. Res. 58 (2019) 23380

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how can we enhance heat transfer?

heat containment

electrification

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how can we do even better?

microwave

induction

heating from the inside

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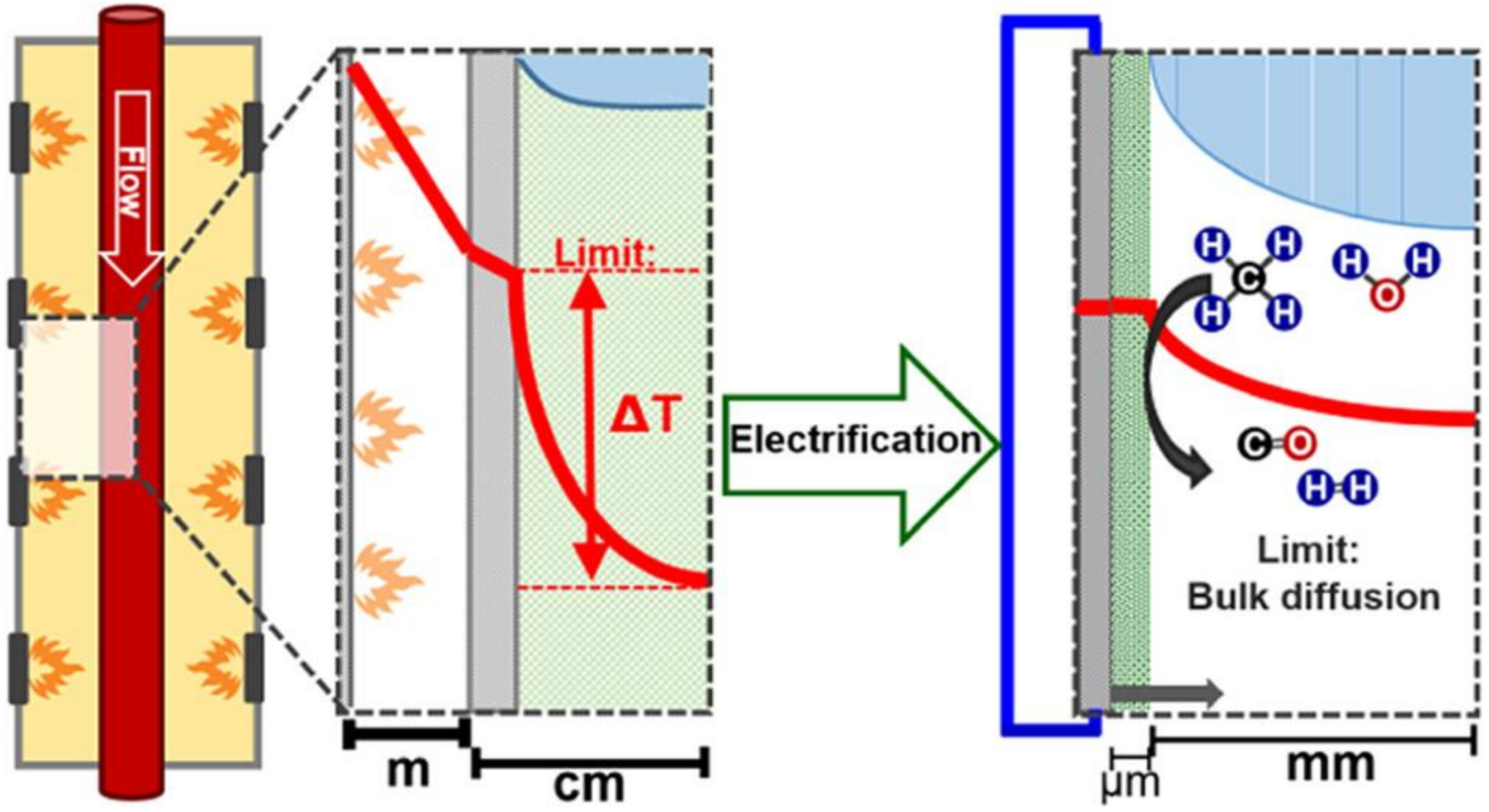
reactor electrification

electrical heating -> overcoming limitations of combustion in furnaces

advantageous in terms of:

- energy efficiency
- process control
- safety and maintenance
- rapid heating
- …



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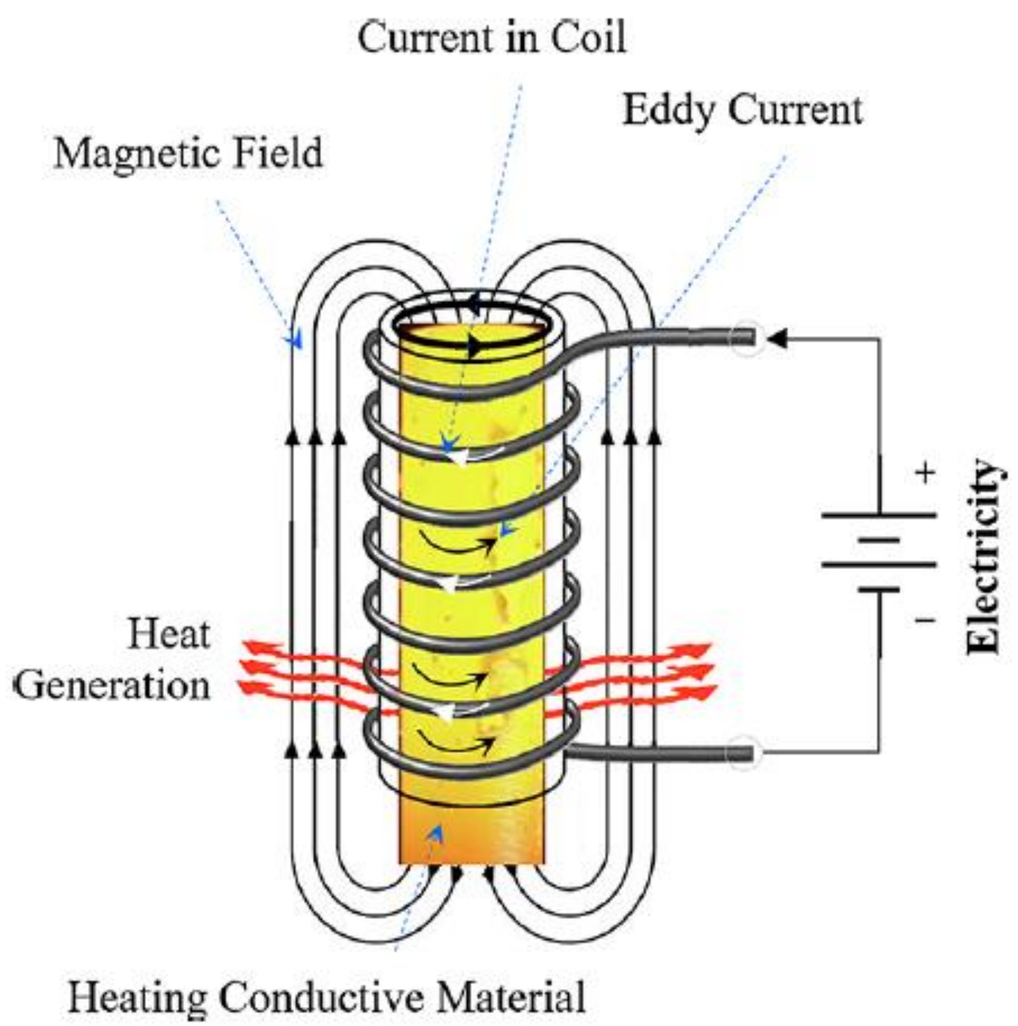
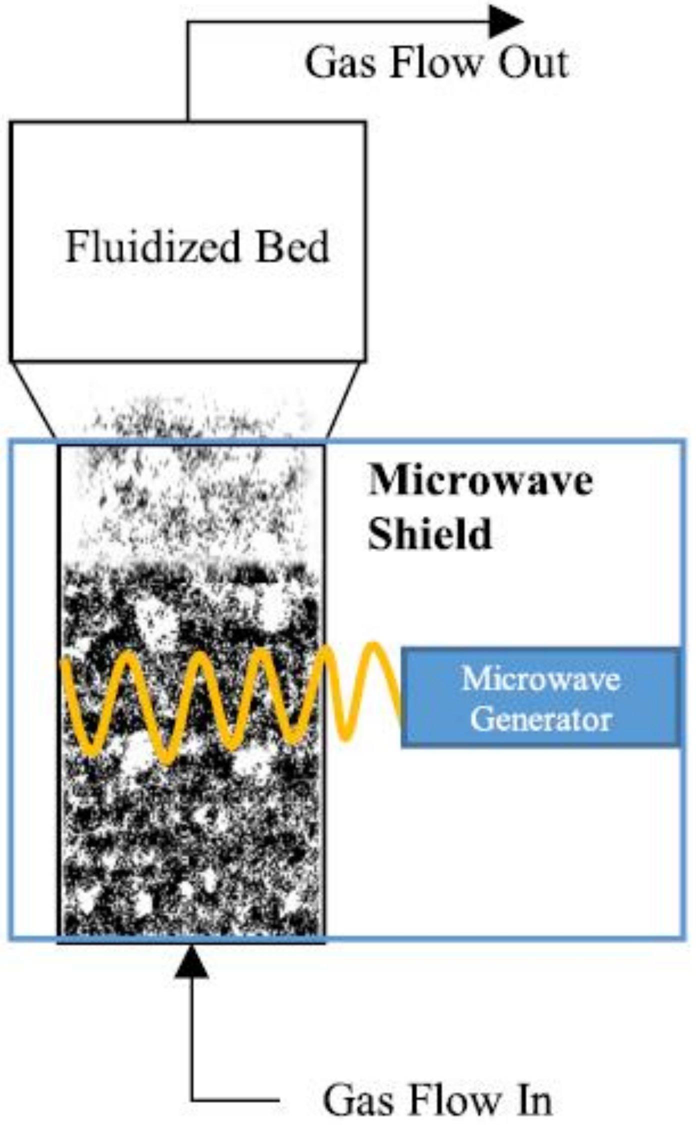
electrical heating

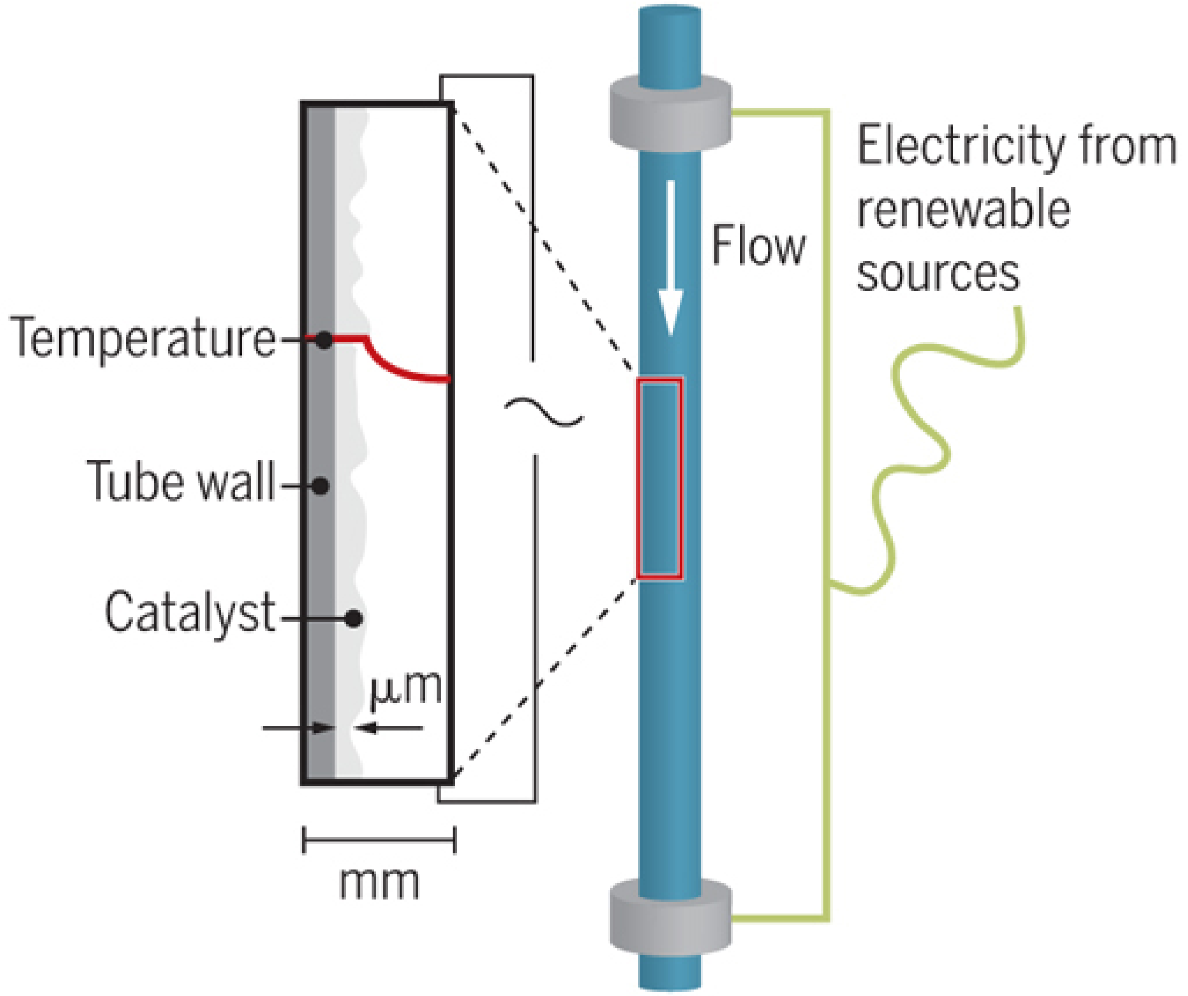
induction



microwave



Joule



Imtiaz, et al. Ind. Eng. Chem. Res. 63 (2024) 4205

sonication
plasma

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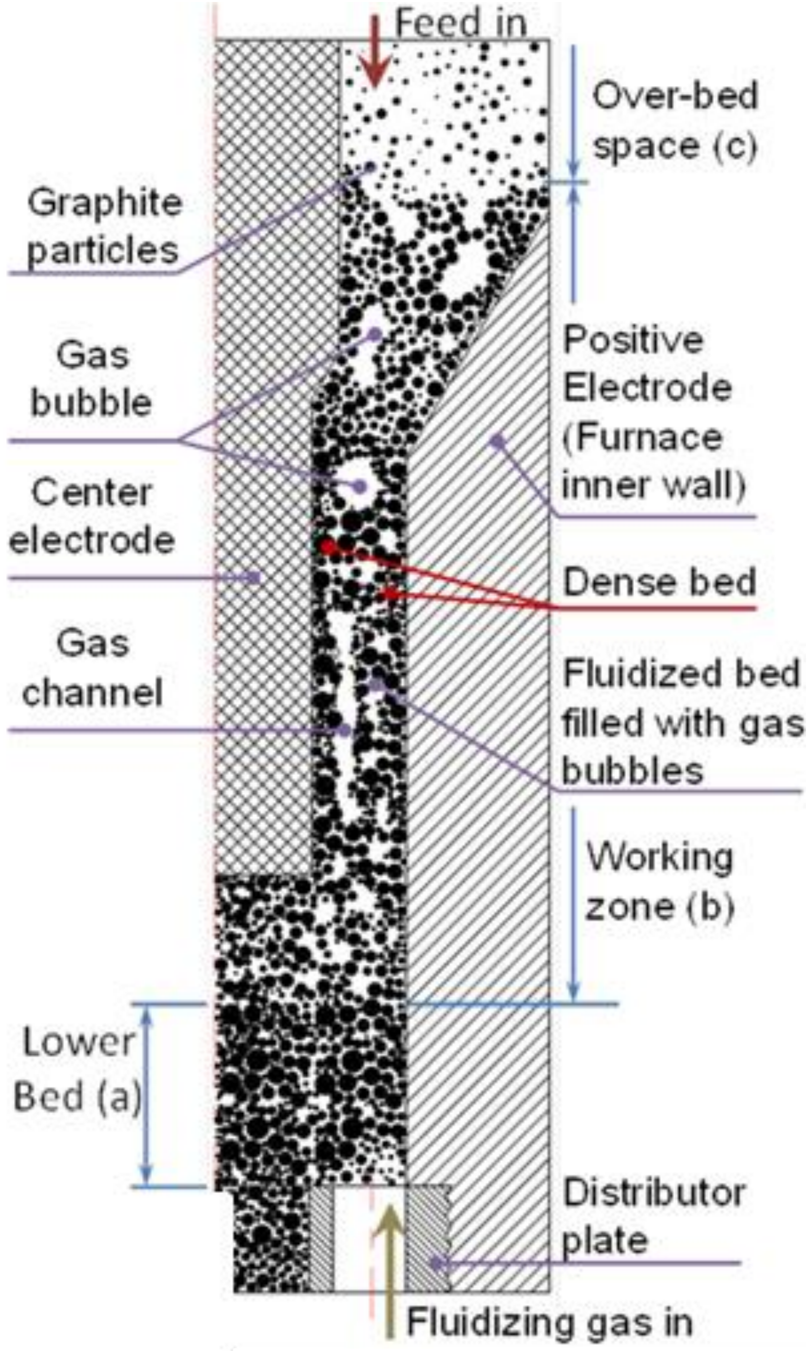
ElectroThermal Fluidized Bed reactor (ETFB)

- combination:
  - fluidization
  - Joule heating
- compared to conventional fluidized beds
  - better control over bed temperature
  - highly energy efficient
  - rapid and uniform heating



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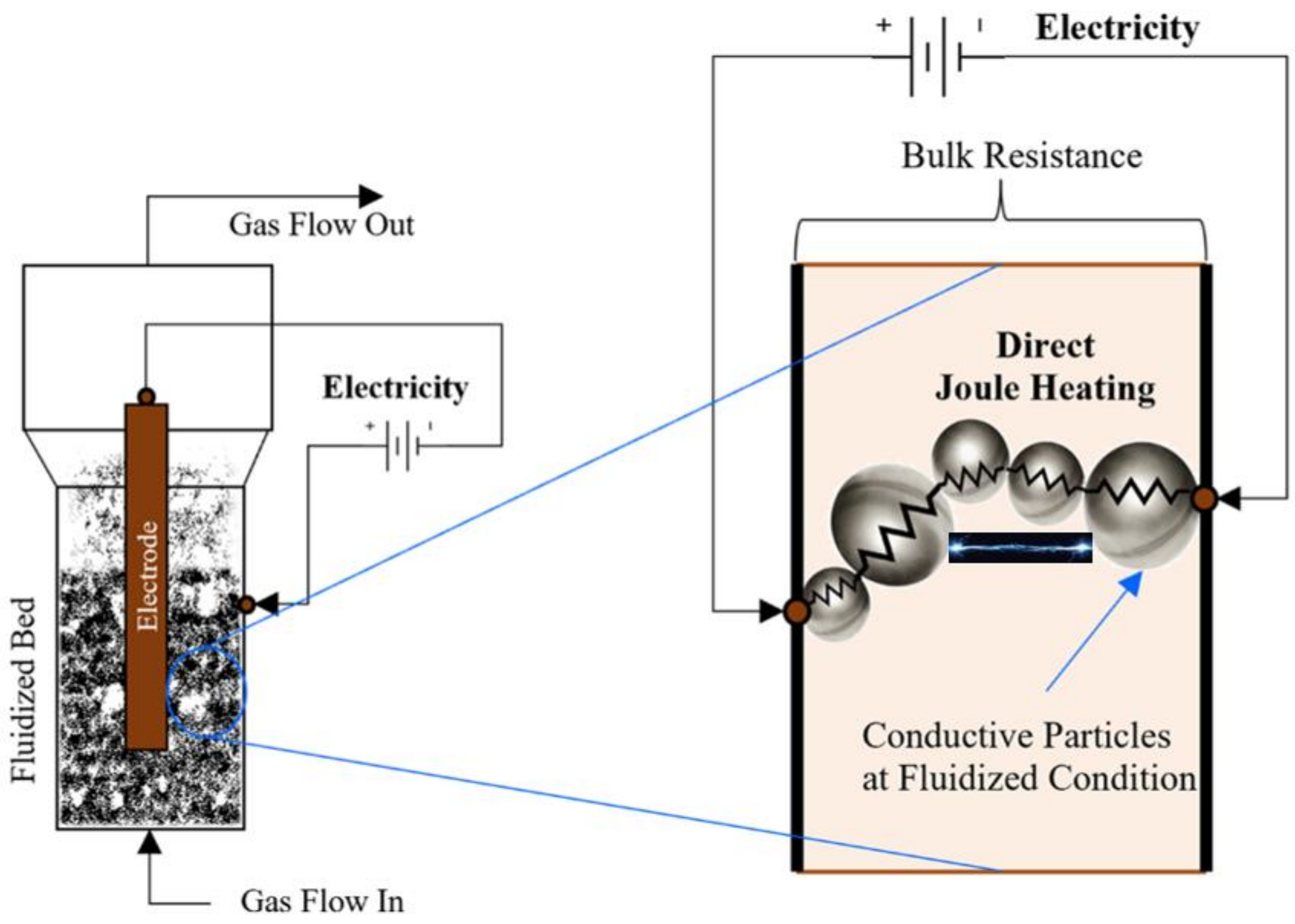
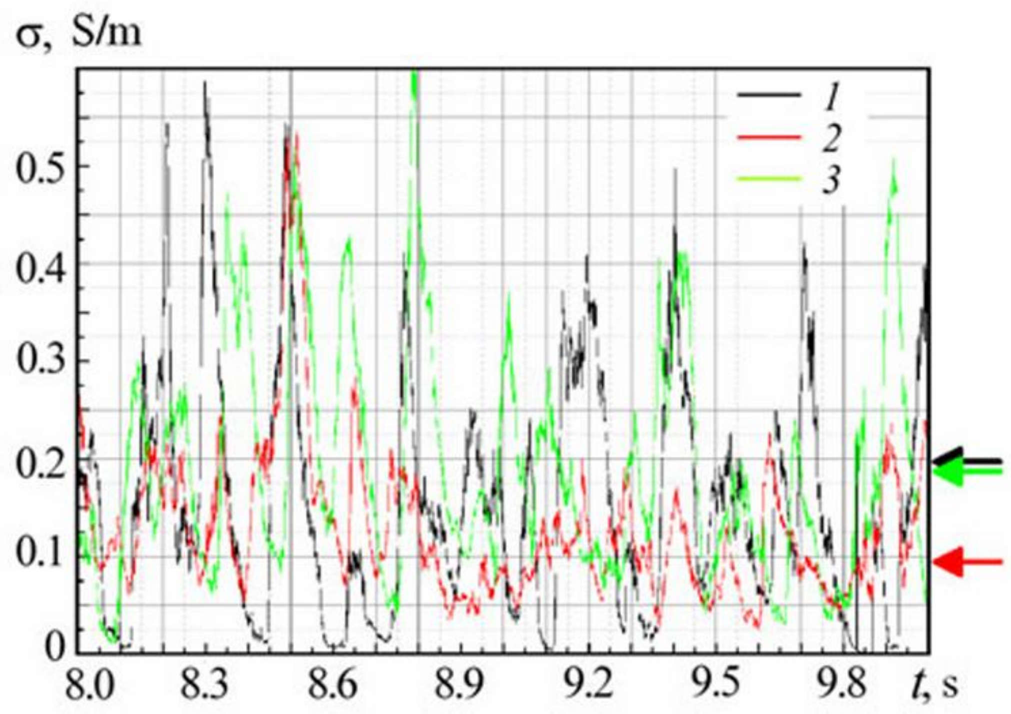
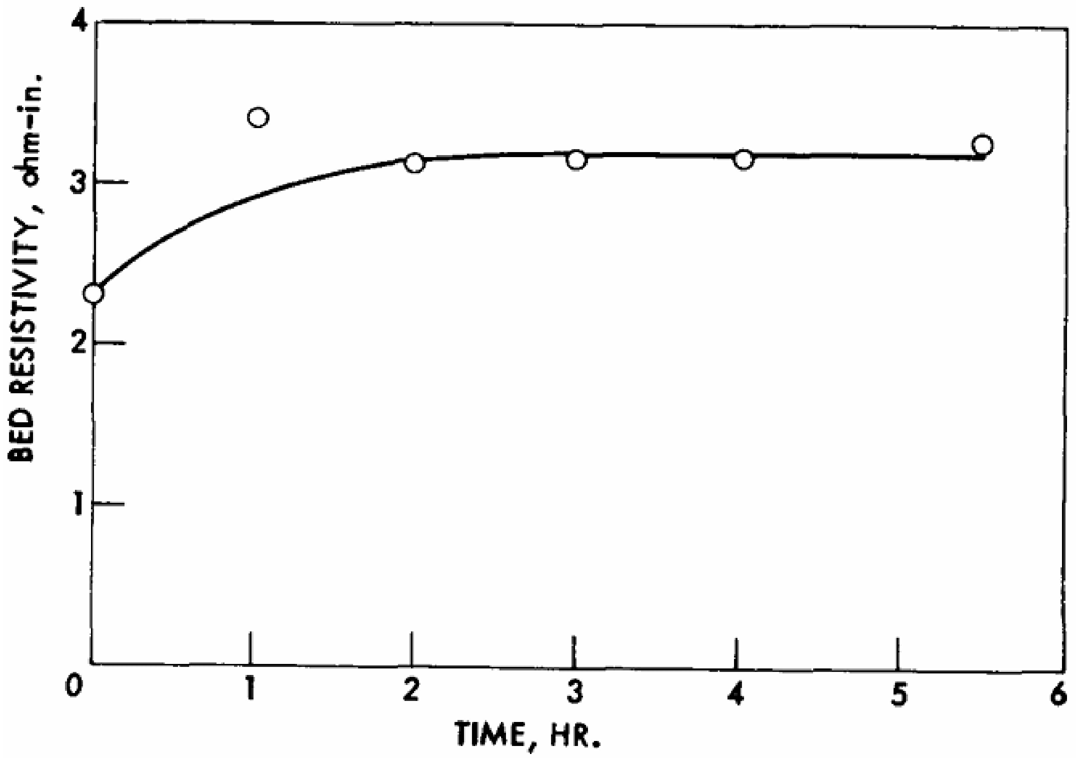
TMEC

Fedorov J. Fluids Eng. 138 (2016) 044502

Joule heating in a fluidized bed







Imtiaz, et al. Ind. Eng. Chem. Res. 63 (2024) 4205

Malinovskii et al., J. Eng. Physics Therm, 85(2), 251–258, 2012

ETFB reactor mass balance

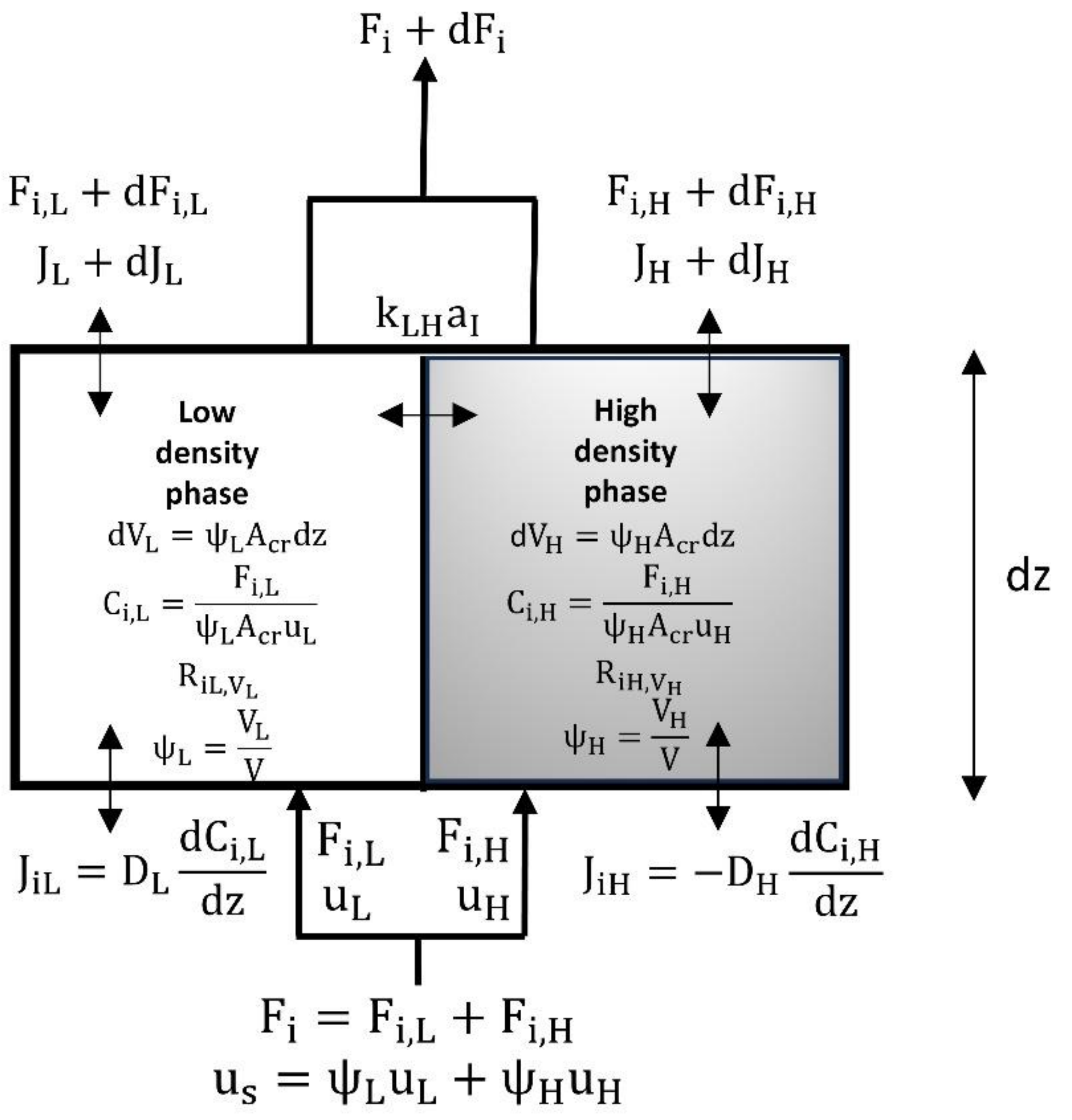
$$\frac{dF_{iX}}{dz} - \varepsilon_X R_{iX,V_X}\psi_X A_{cr} - \frac{D_X}{u_X}\frac{d^2F_{i,X}}{dz^2} + k_{LH}a_I\psi_L\left(\frac{F_{iX}}{\psi_X u_X} - \frac{F_{iY}}{\psi_Y u_Y}\right) = 0$$

convection reaction diffusion phase transfer

X= L/H
Y=H/L

assumptions

- bubbling fluidization regime
- low- and high-density phases are at the same temperature
- no radial profiles
- constant effective conductivity at average temperature and composition
- adiabatic operation
- steady state operation



Jacobs et al. Chem. Eng. Sci. 2026 327 123647

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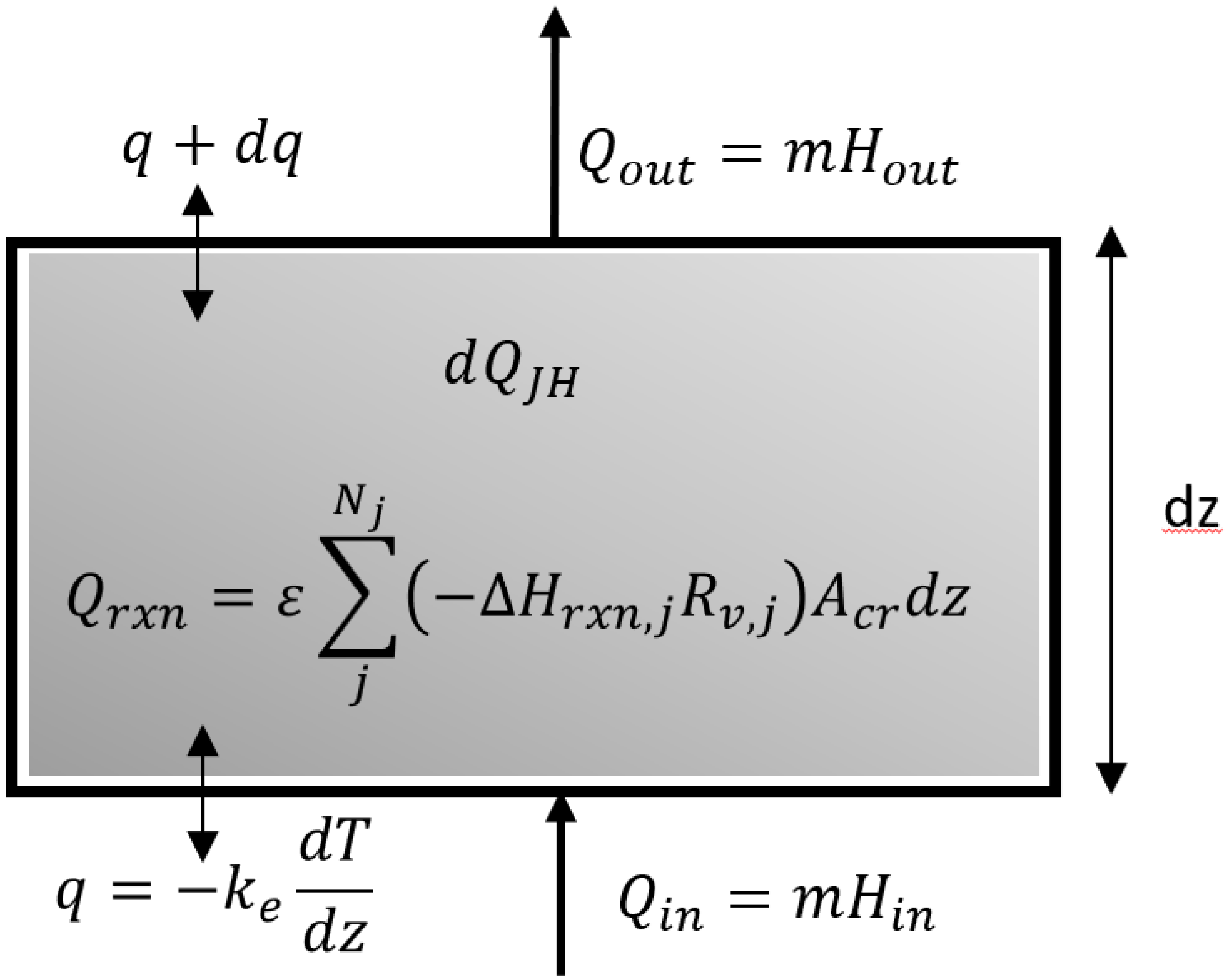
ETFB reactor heat balance

$$u\rho_g C p_g \frac{dT}{dz} - k_e \frac{d^2T}{dz^2} - \varepsilon \sum_j^{N_j} (-\Delta H_{rxn} R_{v,j}) - \frac{\boldsymbol{dQ_{JH}}}{\boldsymbol{dzAc_{reactor}}} = 0$$

convection conduction heat of reaction heat generation
→ Joule heating term



electrical field calculation

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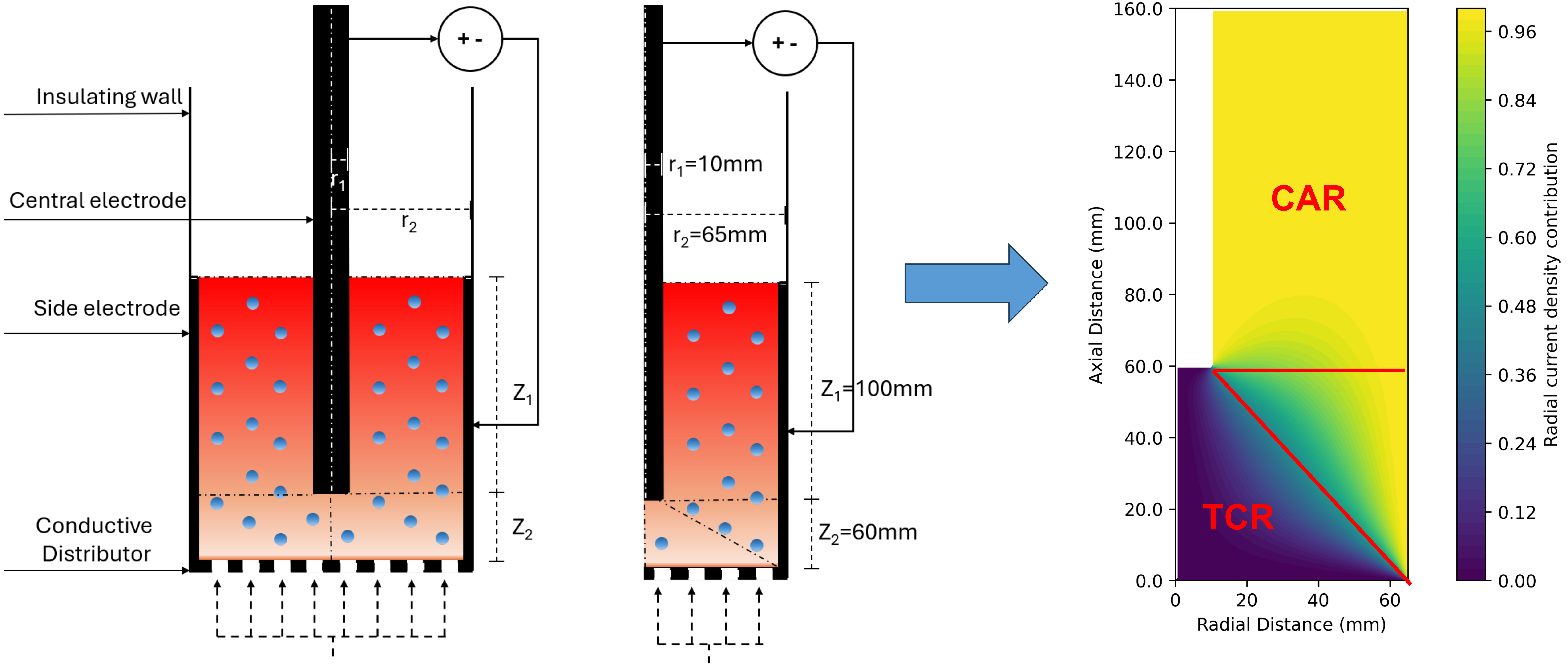
ETFB electrical field

coaxial resistor



truncated cone resistor

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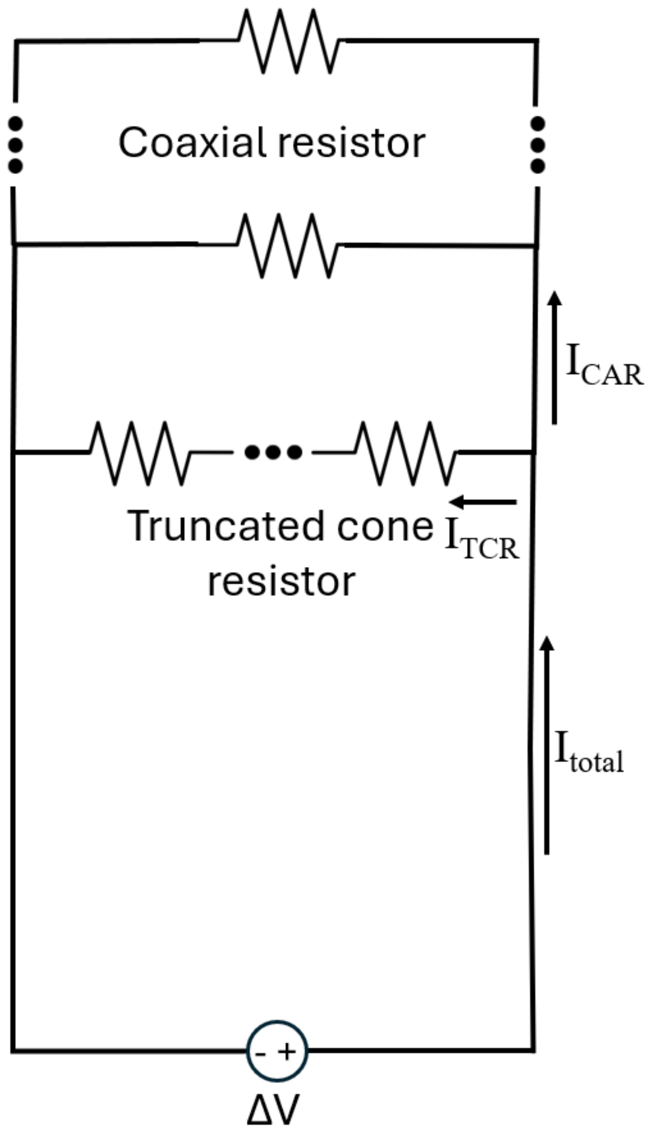
ETFB resistance

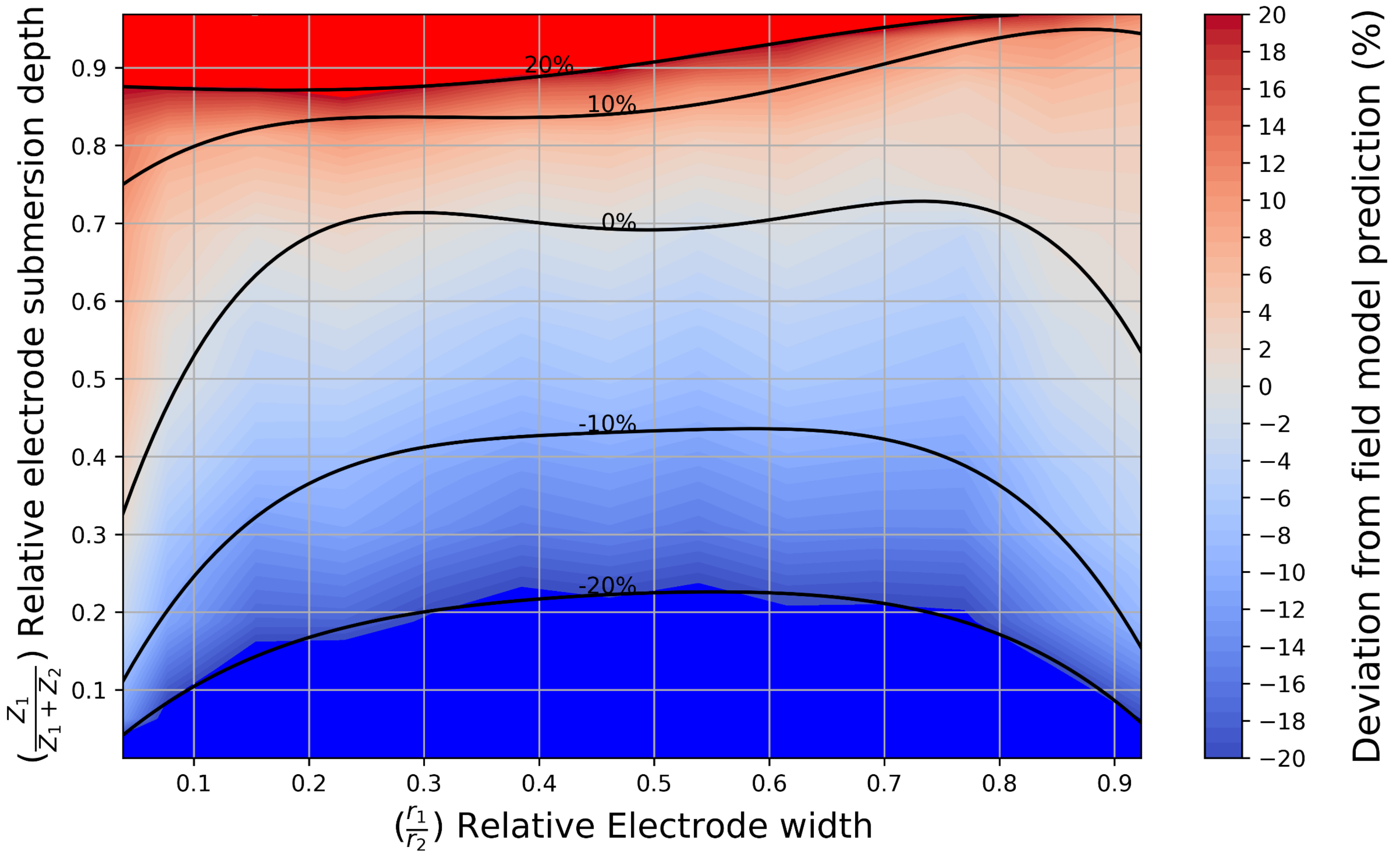
assuming contact resistances with the electrodes are negligible

CARs and TCRs are represented as two resistors in parallel

$$R_{total} = \left(\frac{1}{R_{CAR}} + \frac{1}{R_{TCR}}\right)^{-1}$$

$$Q_{JH,total} = \frac{V^2}{R_{total}} = I_{total}^2 R_{total} = V I_{total}$$





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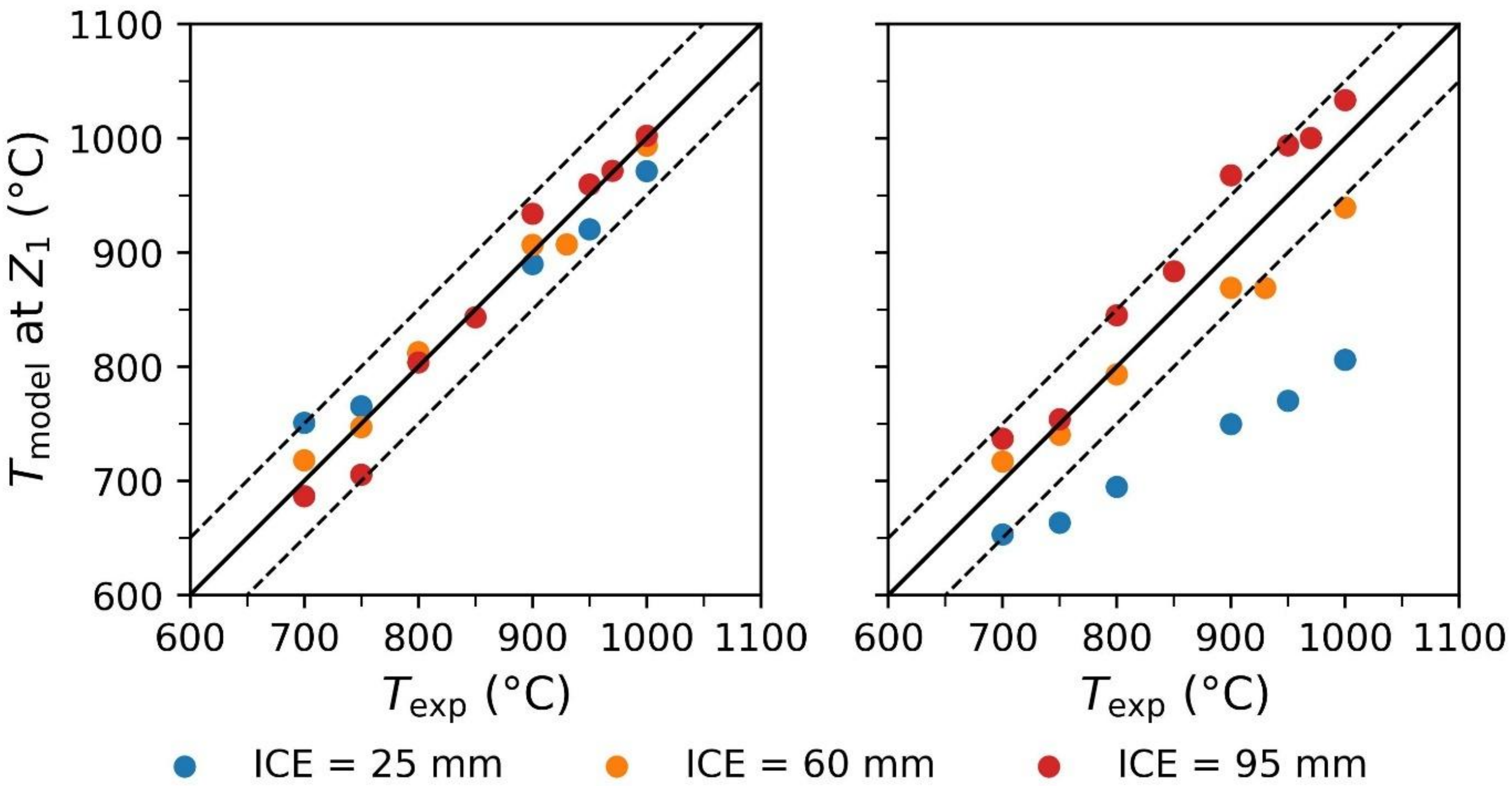
thermal model validation



Ahmed et al. Metal. Mat. Trans. B 2025 56 7150–7166
Jacobs et al. Chem. Eng. Sci. 2026 327 123647

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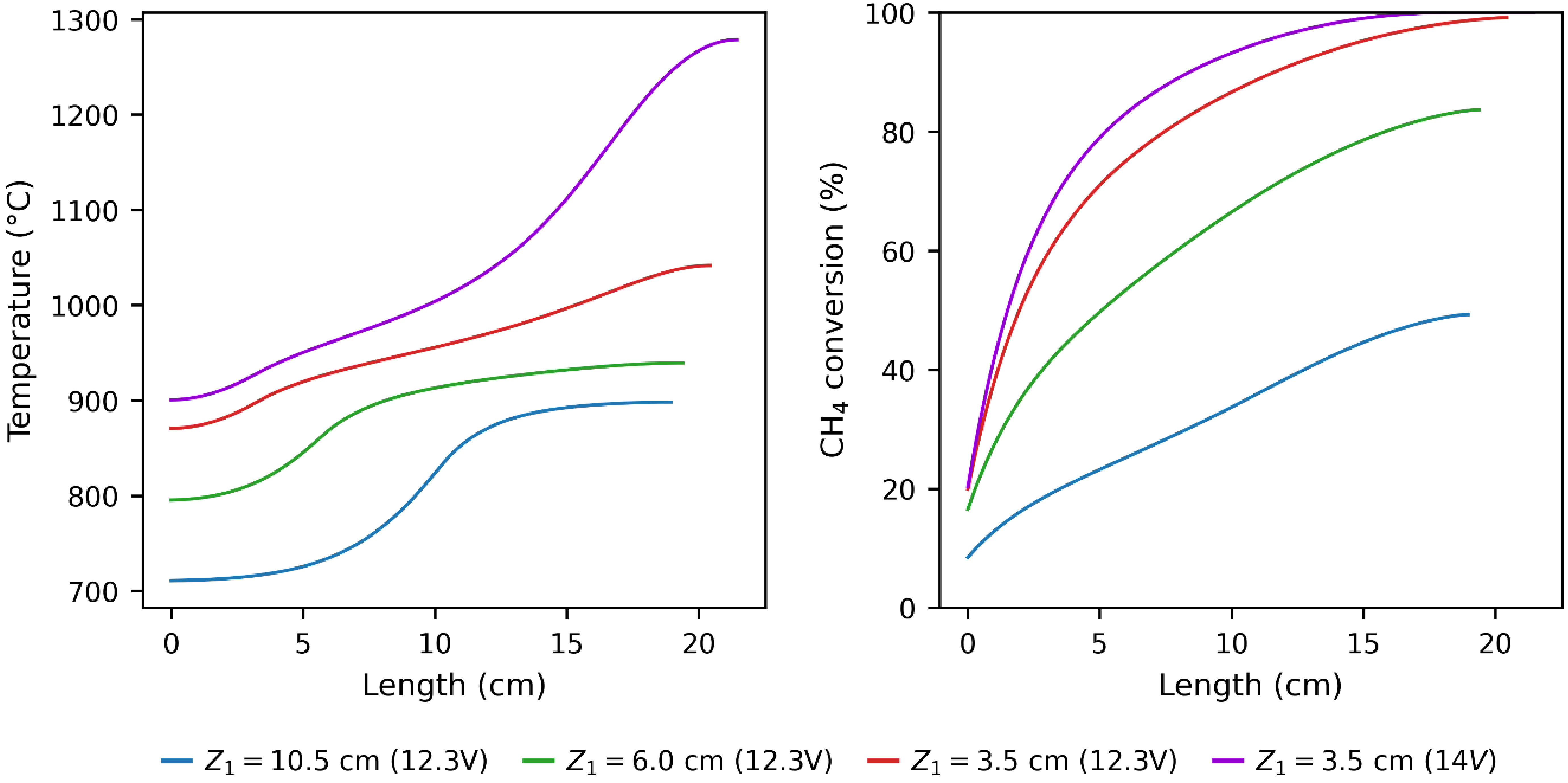
methane pyrolysis performance simulation



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Zareghorbaei et al. Chem. Eng. Proc. PI 2026 submitted

ETFB reactor set-up

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conclusions and perspectives

- "electricity is in the catalyst"
  - reactor electrification not just connecting electric heater to the grid
  - reasoning from the inside: ElectroThermal Fluidized Bed (ETFB) reactor
  - opportunities for endothermic reactions

- methane pyrolysis
  - crucial role of surface area: it increases H radical formation (and methyl radical formation in the gas phase)
  - higher hydrogen purity already at lower temperatures
  - higher temperature/higher space time required to compensate for deactivation

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conclusions and perspectives

- ETFB reactor
  - electrode submersion enhances heat generation
  - temperature excursions in case of full conversion

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acknowledgments

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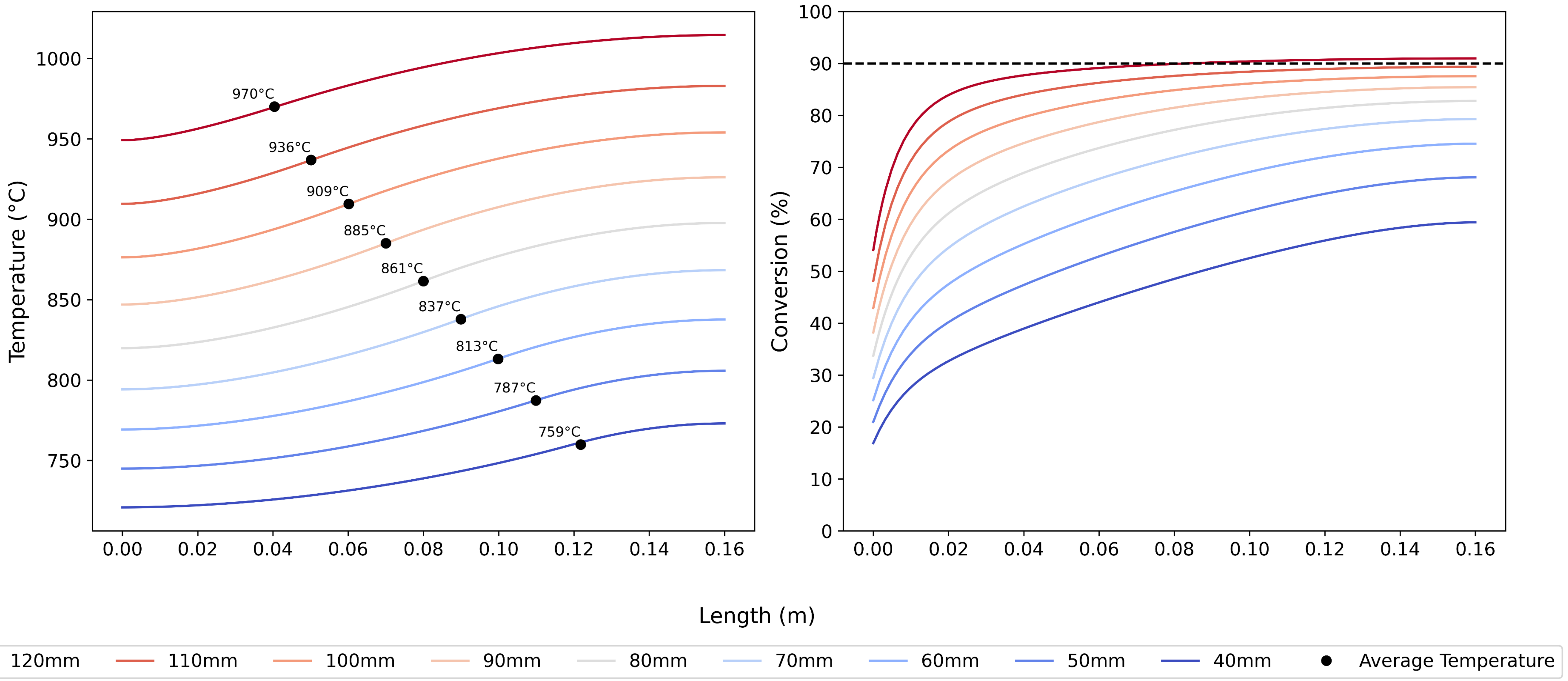
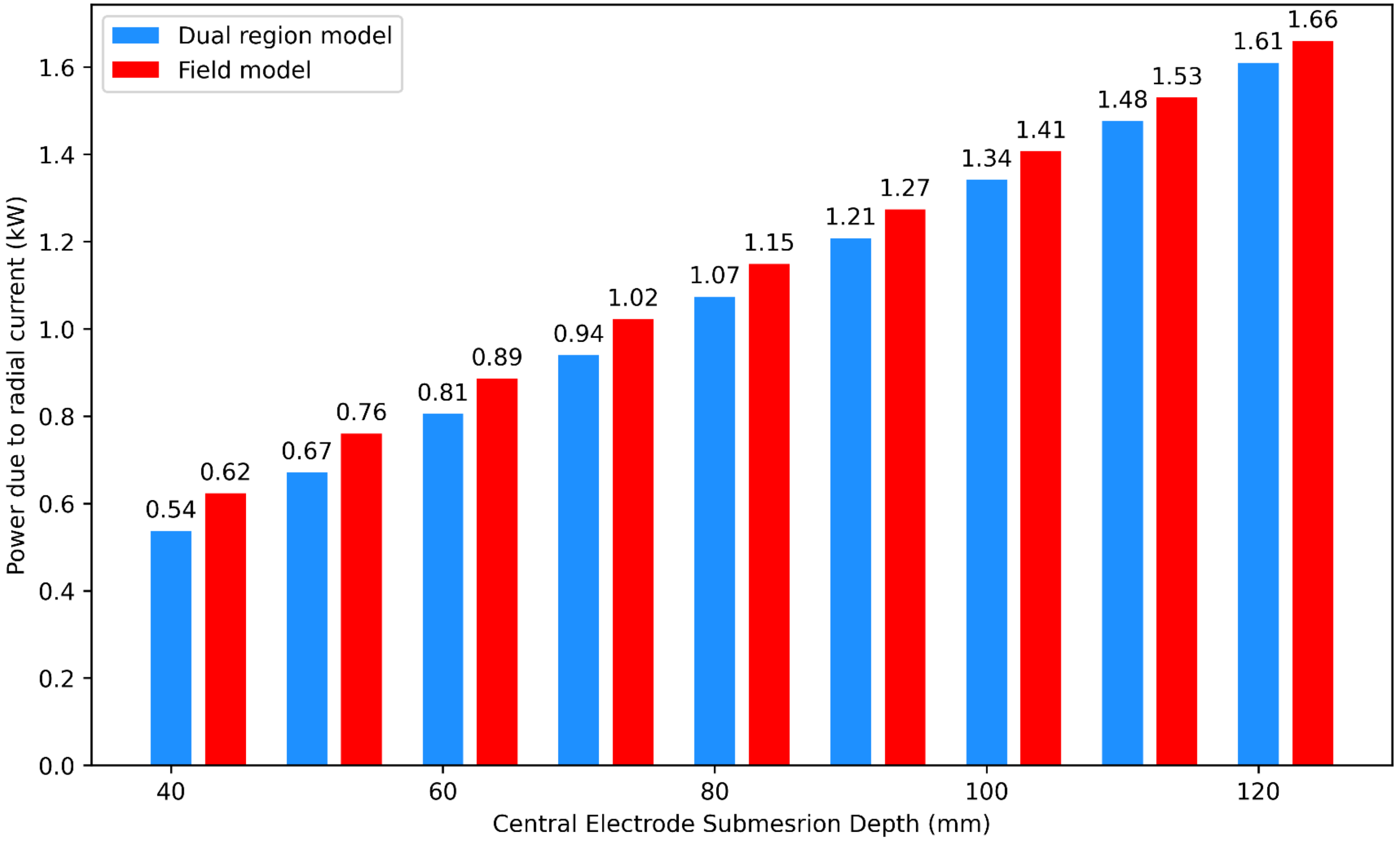
e-CODUCT – ETFB simulation

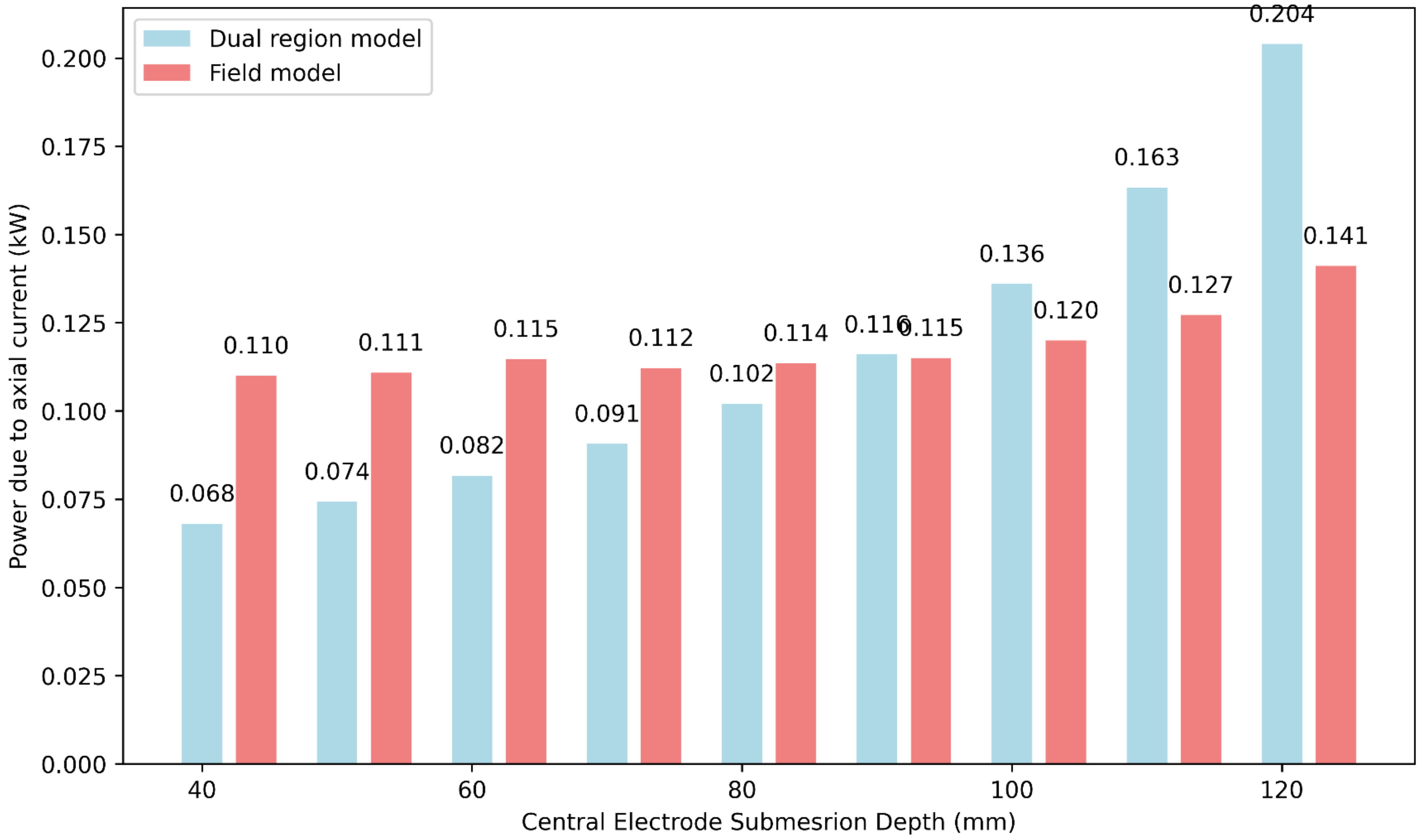


axial temperature (left) and COS conversion (right) profile as function of length for different electrode submersion depth.

2 zone vs field model simulations



coaxial resistor (CAR)



truncated cone resistor (TCR)

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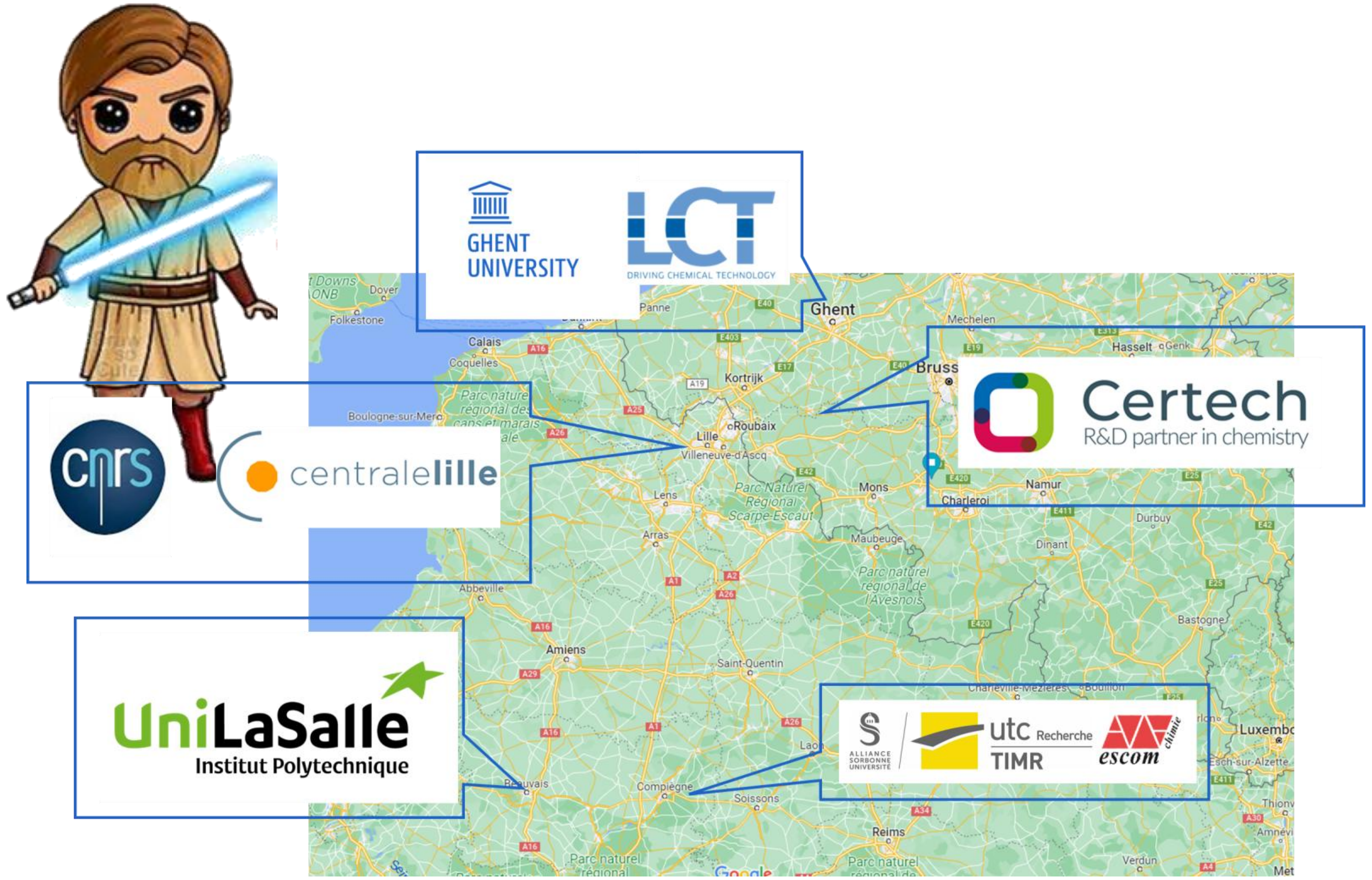
OBIWAN: context

- biogas (CH_4 + CO_2) valorization
  - calorific
  - to chemicals/(sustainable aviation fuels)



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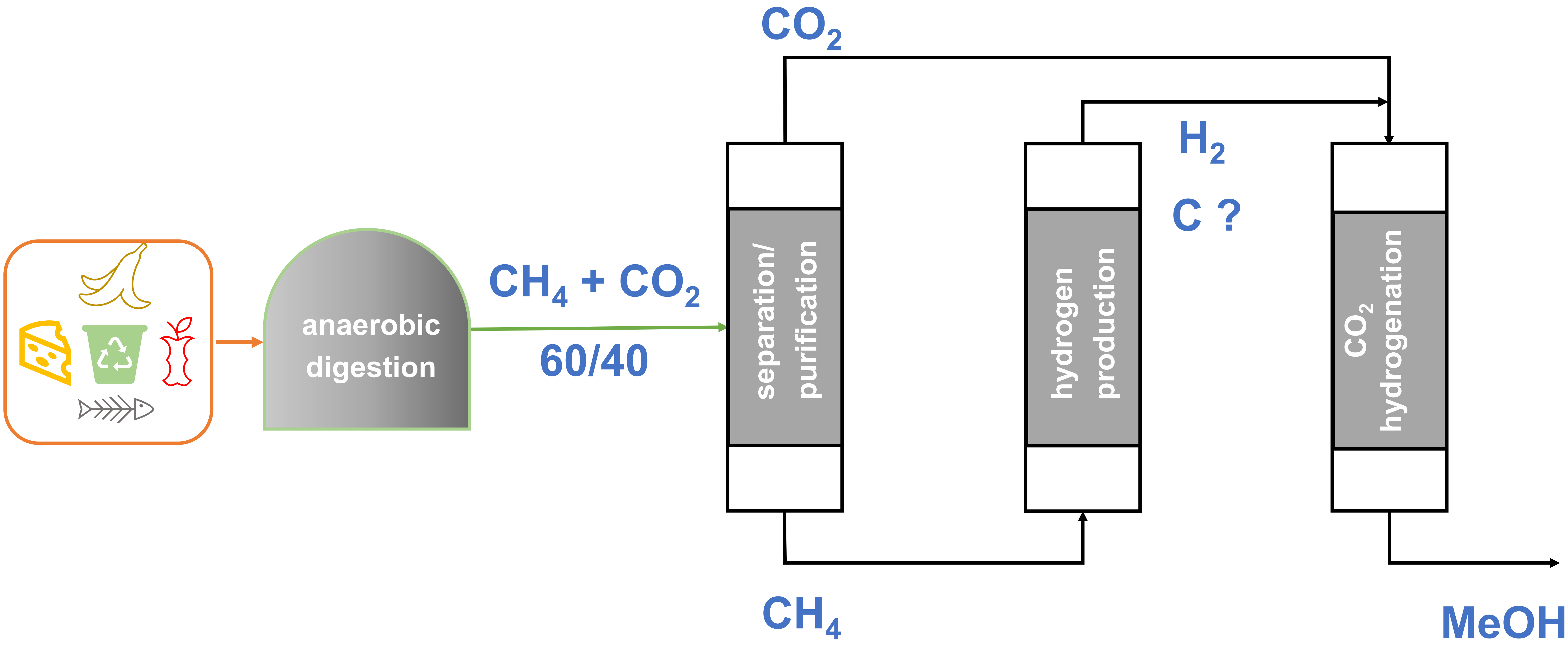
OBIWAN: process lay-out



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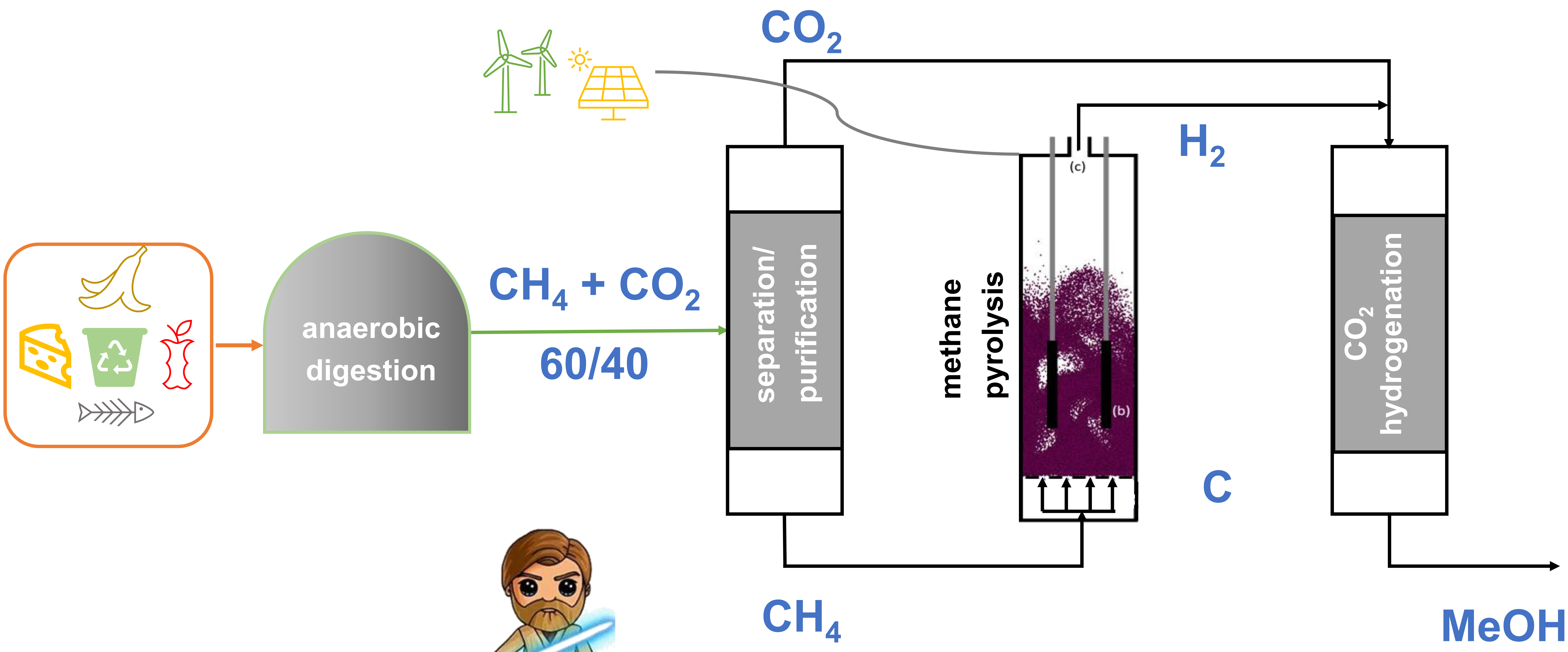
OBIWAN: process lay-out



OBIWAN start: October 2024