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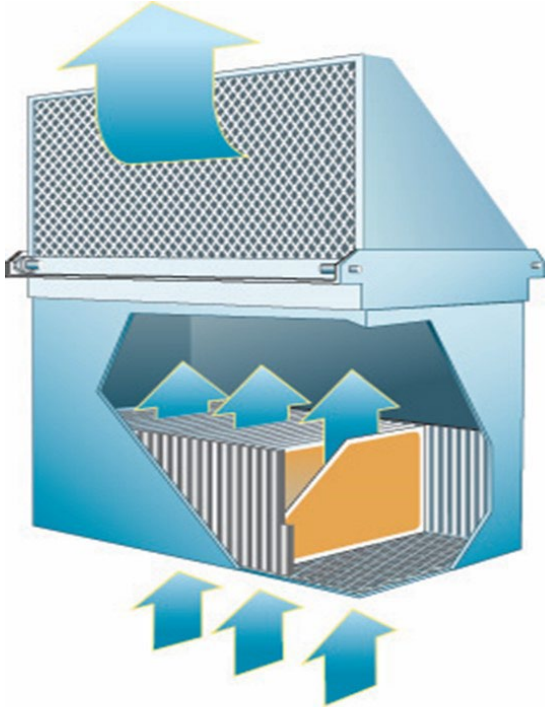
Application of Passive Autocatalytic Recombiners (PARs) for Hydrogen Mitigation: 2D Numerical Modeling and Experimental Validation



ICHS Conference, Quebec City, QC

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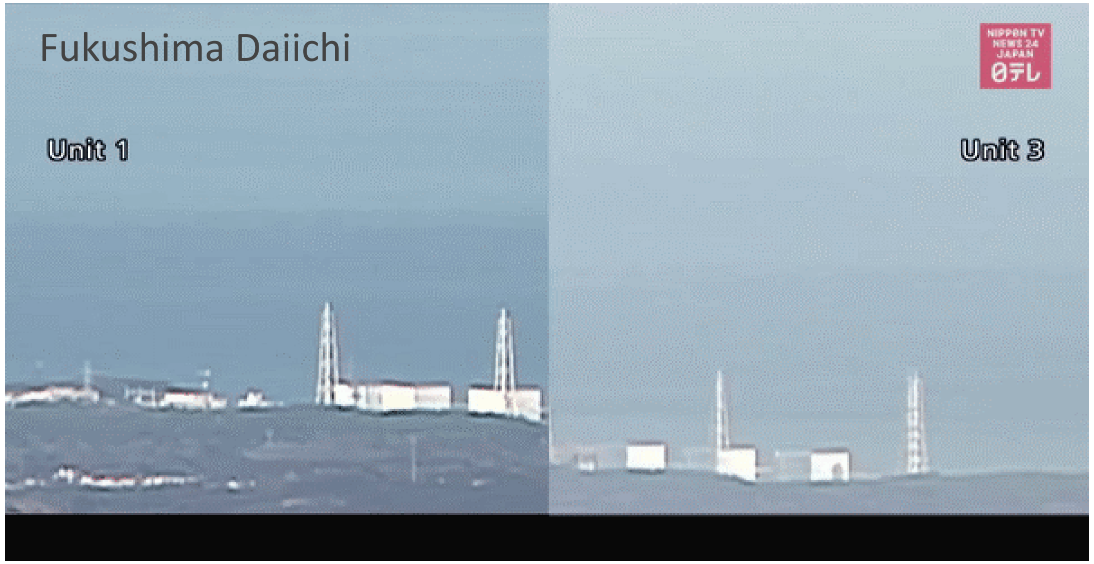
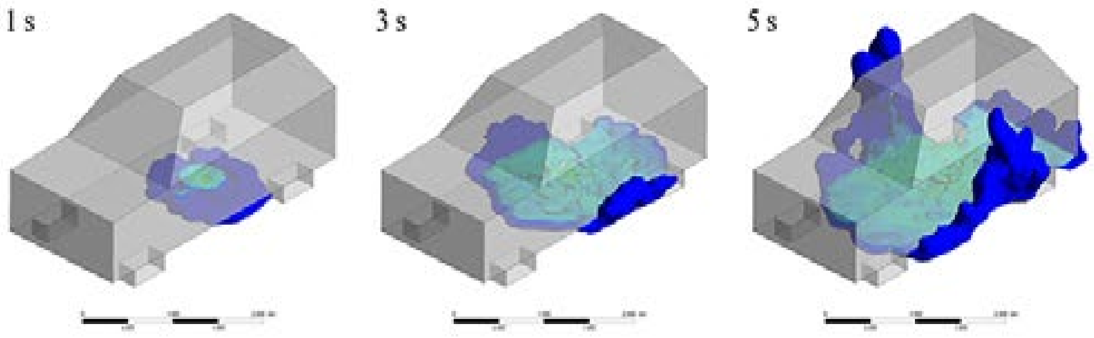
Background: Hydrogen Release

- **Nuclear Context:**
  - Hydrogen (H_2) and carbon monoxide (CO) can be released during a nuclear reactor accident with a loss of coolant:
    - H_2: Hot steam + Zr metal
    - H_2+CO: Molten core concrete interaction
- **Non-Nuclear Context:**
  - H_2 can be released from leaks in H_2 vehicles placed in confined and semi-confined areas: underground mining, parking garages, and road tunnels where CO can be present.





Huang, T., et al., Modeling of hydrogen dispersion from hydrogen fuel cell vehicles in an underground parking garage. International Journal of Hydrogen Energy, 2022. 47(1): p. 686-696.

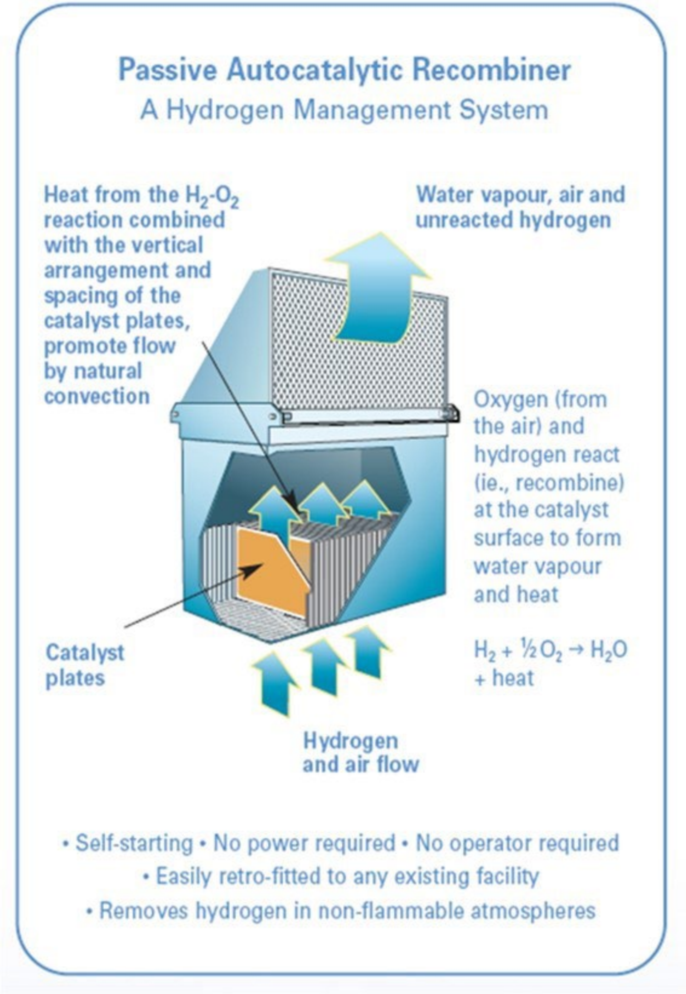
Hydrogen Mitigation

- **Both Contexts:**
  - ➢ Hydrogen accumulation could create a flammable mixture:

    - Ignition → Fire/explosion:

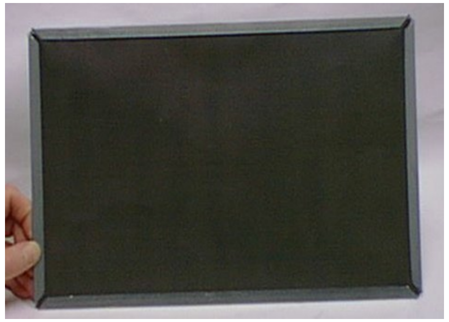
      → threat to structures and life.

- **Hydrogen Mitigation Measures**
  - ➢ Large free volume → dilution of H_2.
  - ➢ Ventilation (non-nuclear context).
  - ➢ Active or Passive Autocatalytic Recombiners.



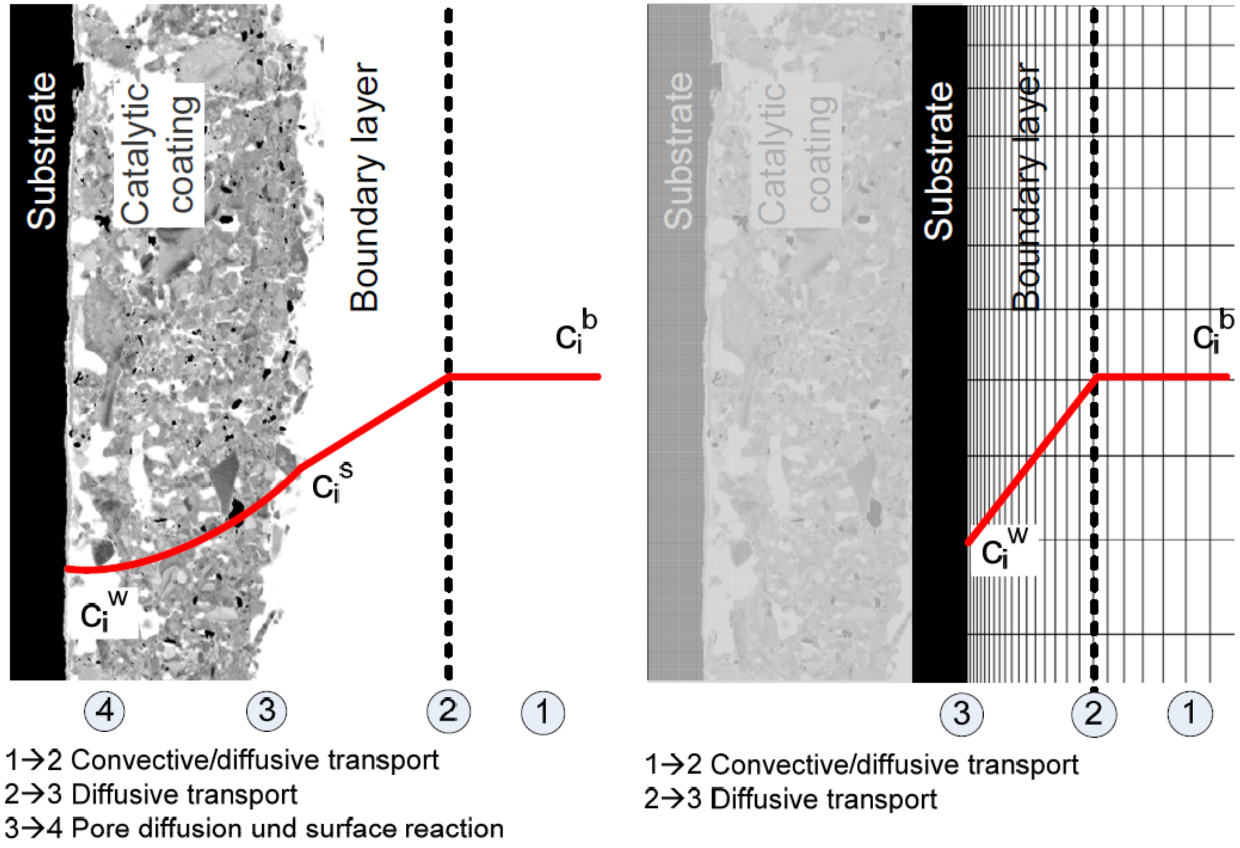
PAR

Catalyst Plate



PAR Operation

- **Thermochemical Mechanisms:**
  - Species transport from the bulk fluid to the catalyst surface.
  - Surface reactions.
  - Convection of the bulk fluid through the PAR chimney.
  - Heat losses through convection and radiation.
  - Catalyst poisoning (if CO is available).
- **Experiments:**
  - Limited in capturing complex mechanisms.
  - Potentially expensive and time consuming.
- **Numerical Model:**
  - Used to improve the fundamental understanding of such complex mechanisms.
  - Predict the PAR performance in a wide range of conditions.

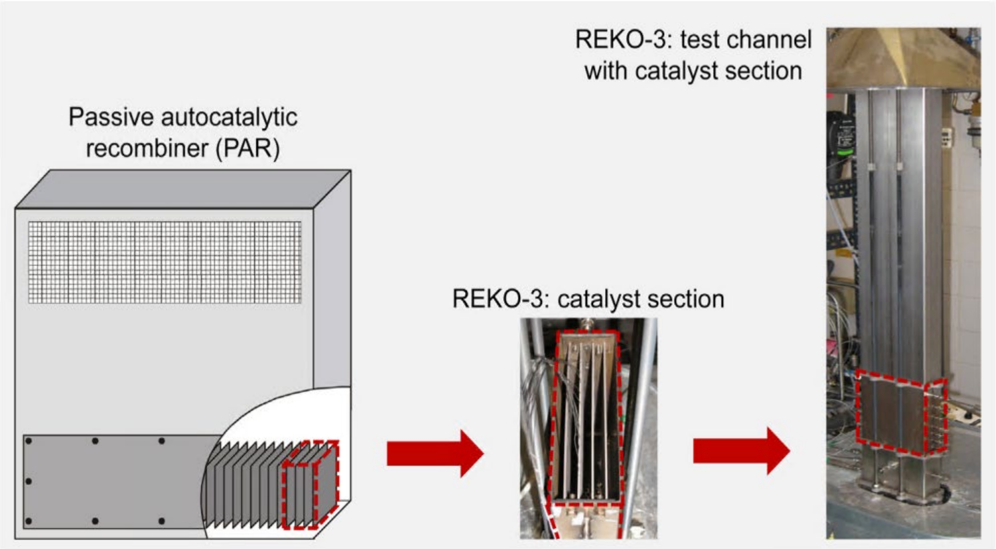


Kelm, S., W. Jahn, and E.-A. Reinecke. *Operational behaviour of catalytic recombiners - experimental results and modelling approaches*. in *Computational Fluid Dynamics (CFD) in Nuclear Reactor Safety (NRS) - Proceedings of the workshop on Experiments and CFD Code Application to Nuclear Reactor Safety (XCFD4NRS)*. 2008. Nuclear Energy Agency of the OECD (NEA).

2D Transient PAR Model: Experimental Setup

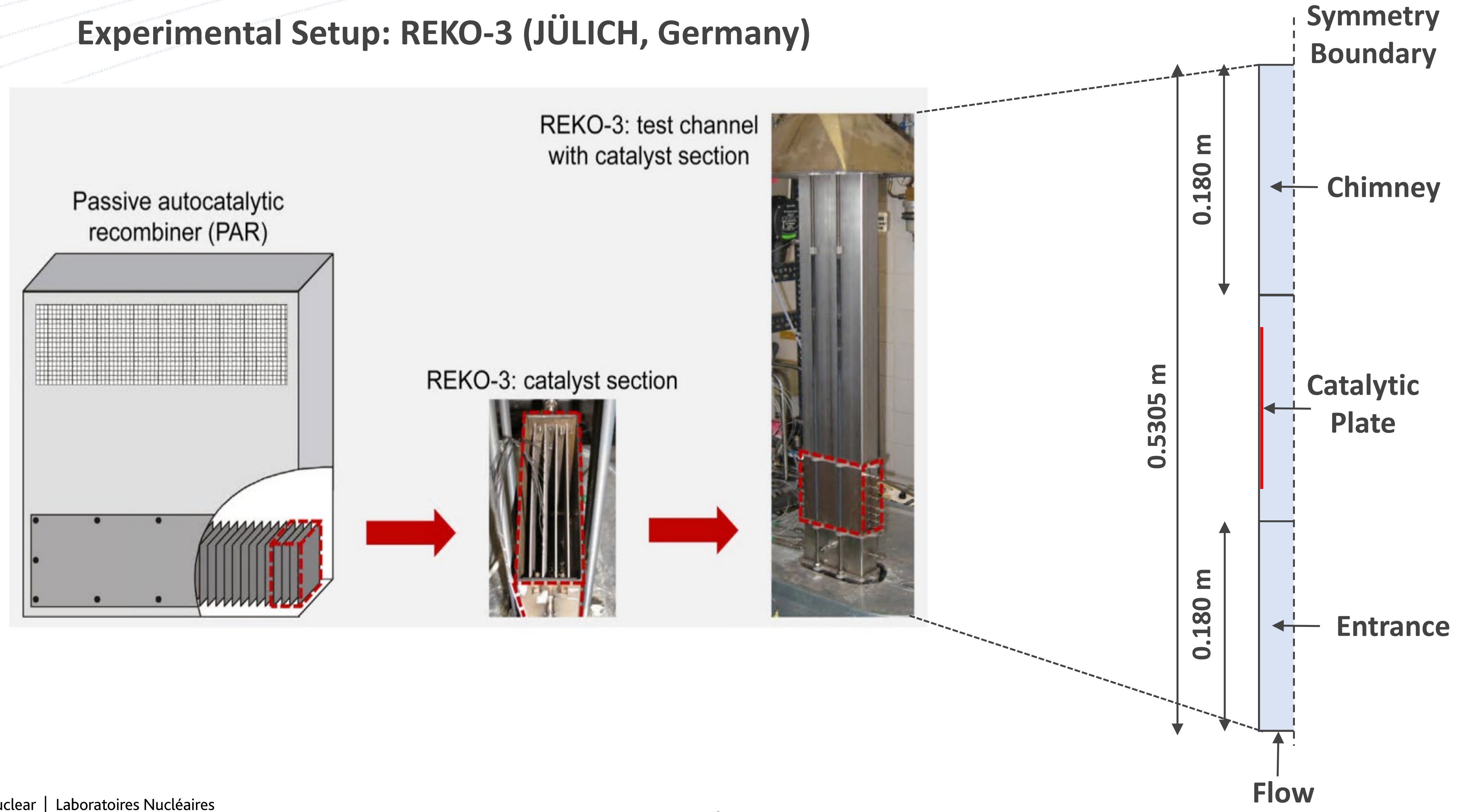
REKO-3 Tests (JÜLICH, Germany)

- H_2-CO steady-state tests.
- Forced flow.
- Different H_2 and CO inlet concentrations.
- Catalyst temperature measurements.
- Gas concentration measurements (inlet and outlet).

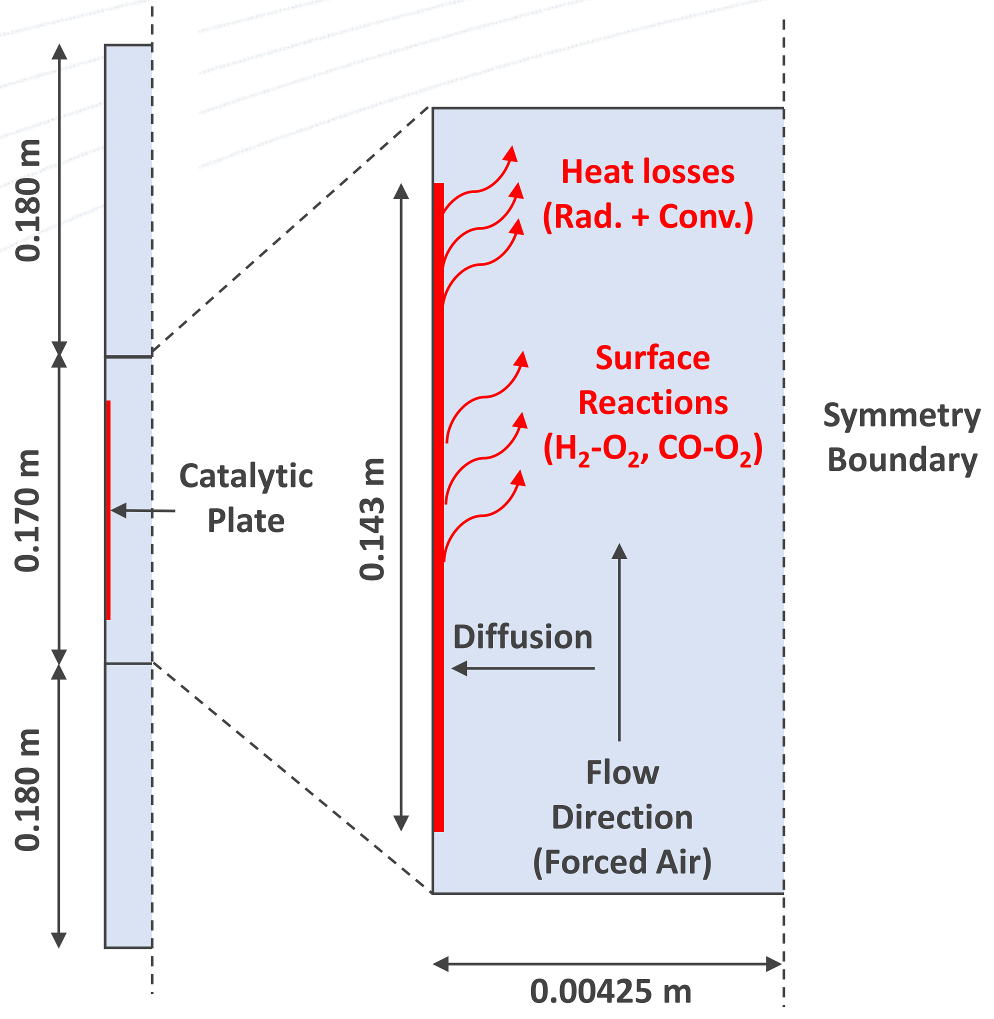


2D Transient PAR Model: Model Geometry

Experimental Setup: REKO-3 (JÜLICH, Germany)



2D Transient PAR Model: Governing Mechanisms



Model Physics

- Forced Laminar flow
- Heat transfer in solids and fluid
- Radiation heat losses
- Transport of species (H_2, O_2, N_2, H_2O, CO, CO_2)
- Surface reactions:

$$H_2 \underset{k^r_{H_2}}{\overset{k^f_{H_2}}{\rightleftharpoons}} H_{2(ads)}$$

$$O_2 \underset{k^r_{O_2}}{\overset{k^f_{O_2}}{\rightleftharpoons}} O_{2(ads)}$$

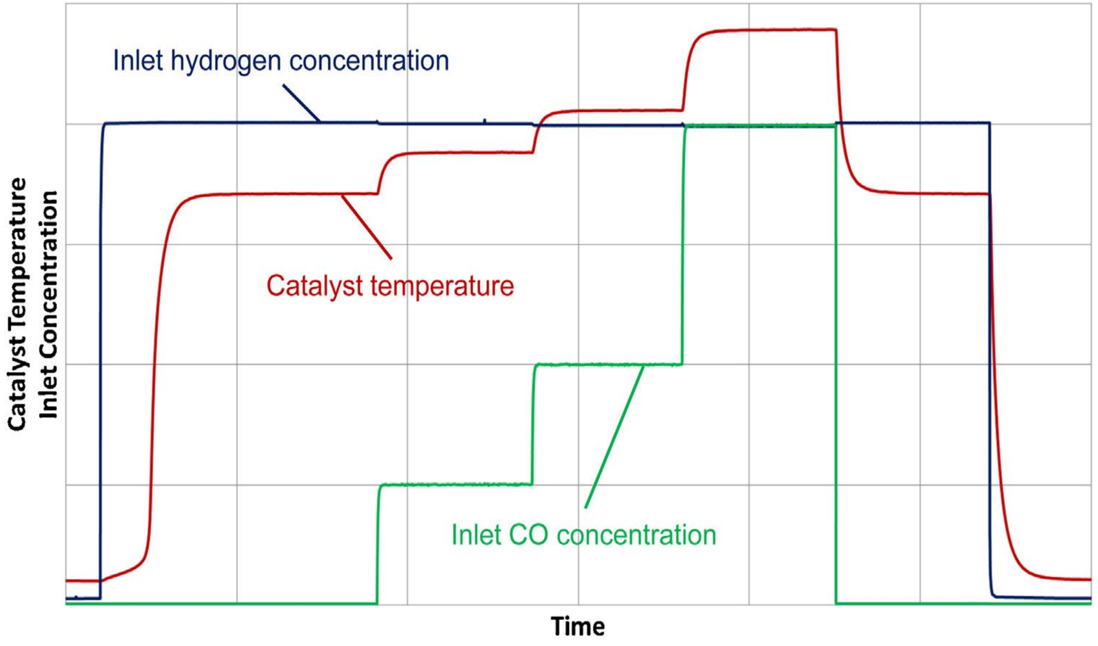
$$CO \underset{k^r_{CO}}{\overset{k^f_{CO}}{\rightleftharpoons}} CO_{(ads)}$$

$$2H_{2(ads)} + O_{2(ads)} \xrightarrow{k_{H_2-O_2}} 2H_2O_{(v)}$$

$$2CO_{(ads)} + O_{2(ads)} \xrightarrow{k_{CO-O_2}} 2CO_{2(g)}$$

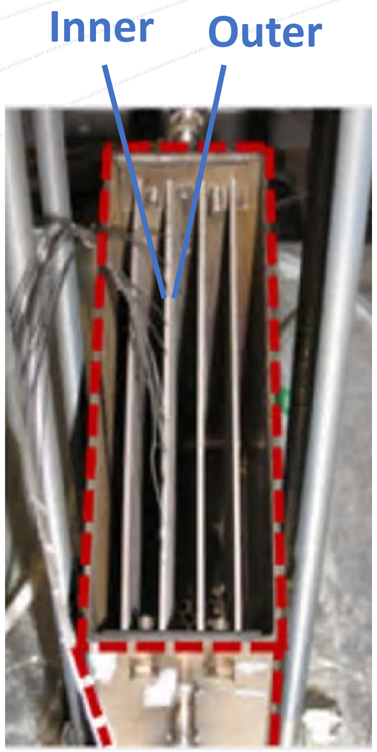
2D Transient PAR Model: REKO-3 Experiments

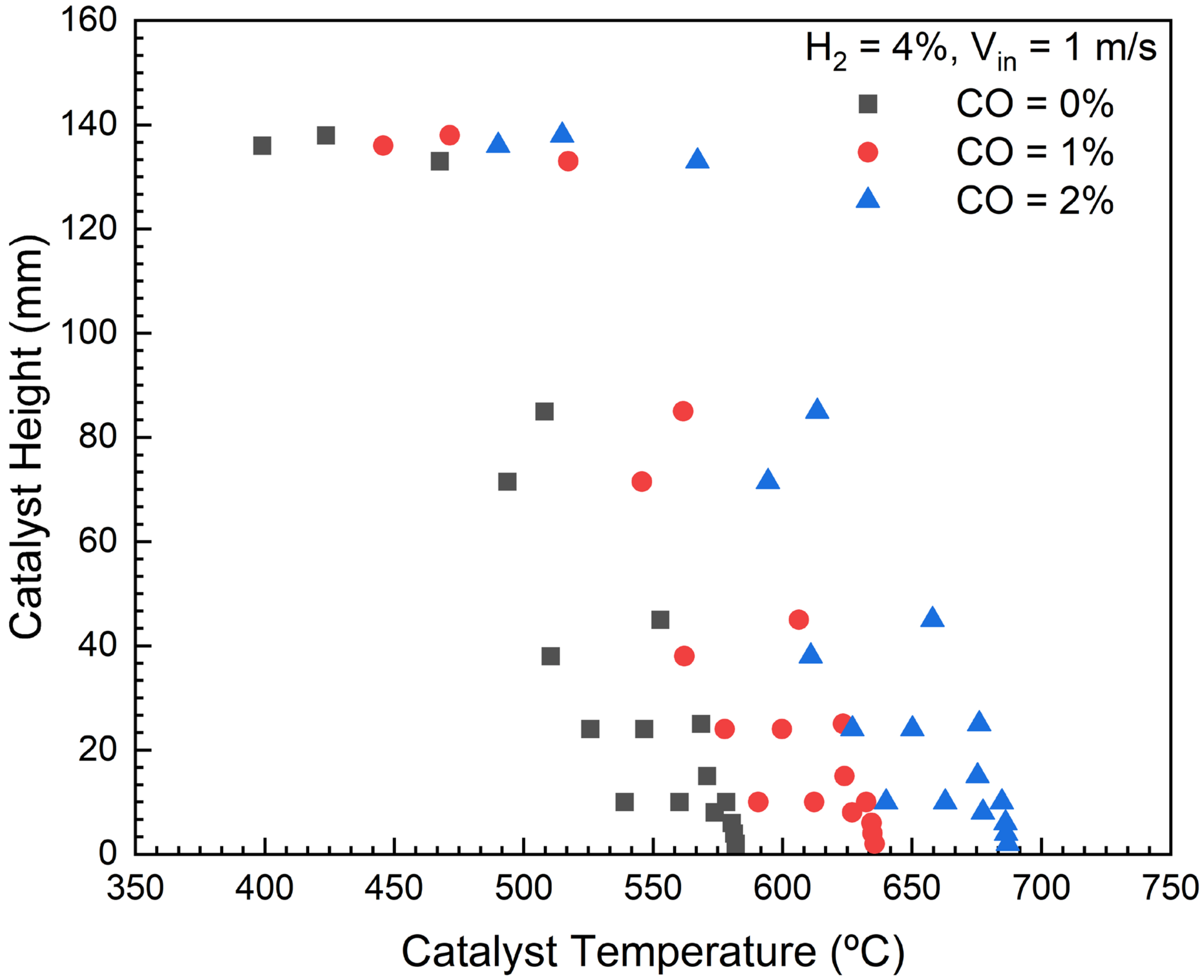
Experiment (#)	Forced Inlet Velocity (m/s)	$H_{2,in}$ (vol.%)	CO_{in} (vol.%)
1	1.0	4.0	0.0
2	1.0	4.0	1.0
3	1.0	4.0	2.0



- H_2-O_2 Calibration
- CO-O_2 Calibration
- Model Validation

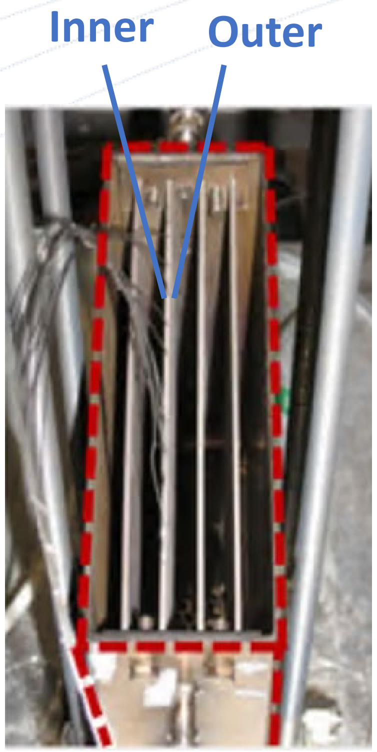
2D Transient PAR Model: Experiments

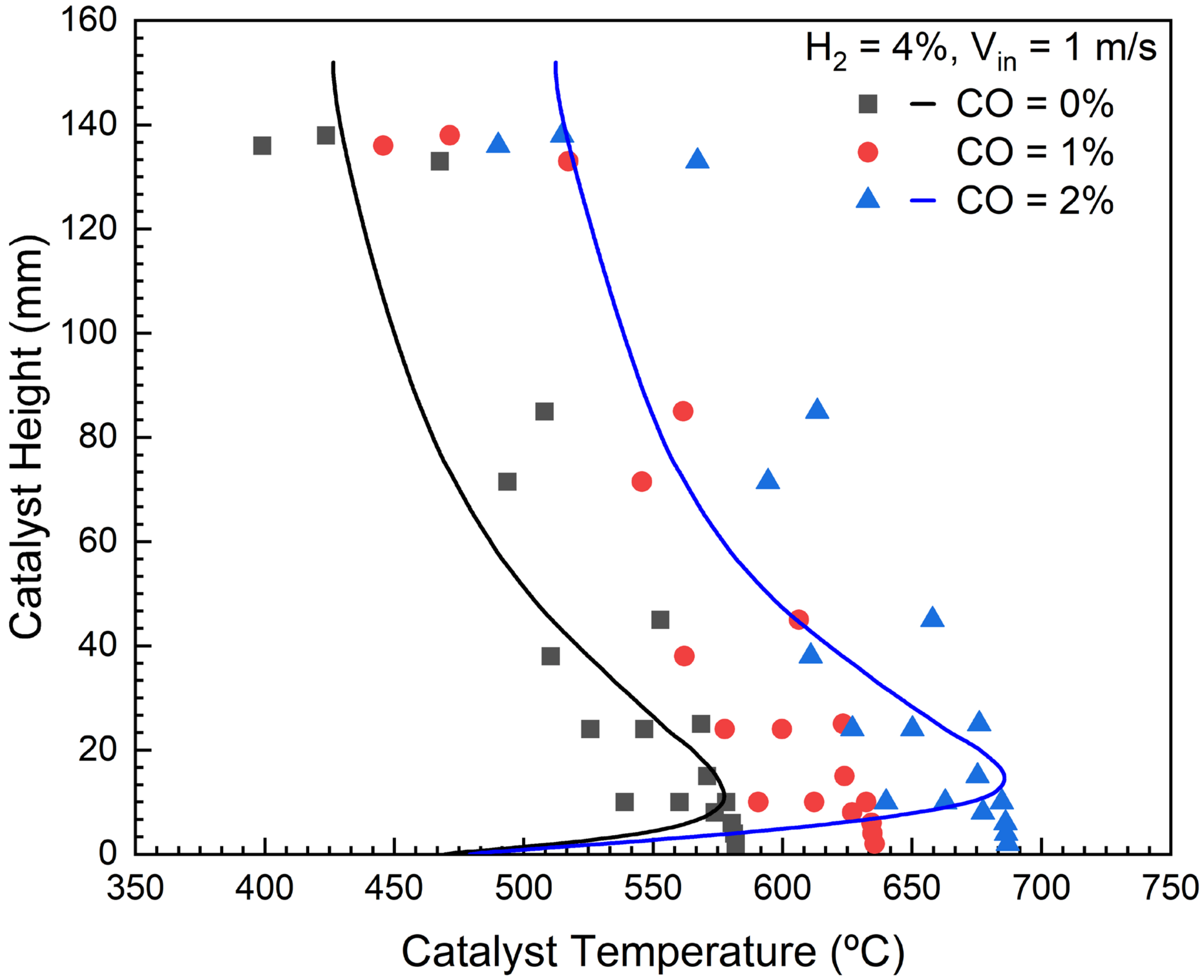




- Plate base: higher temperatures
  - Higher H_2 concentrations
- Plate top: lower temperatures
  - Lower H_2 concentrations
  - Heat losses

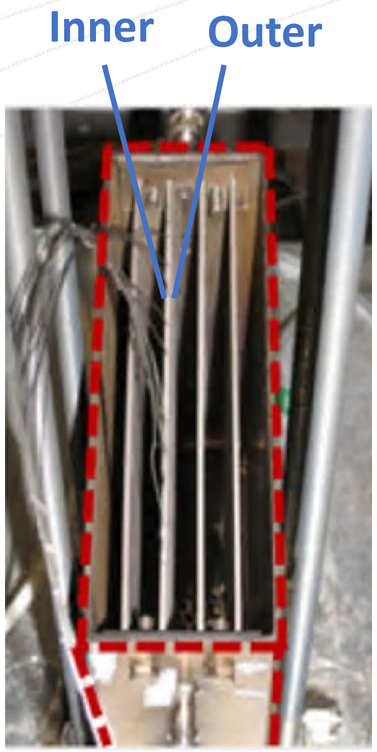
2D Transient PAR Model: Calibration

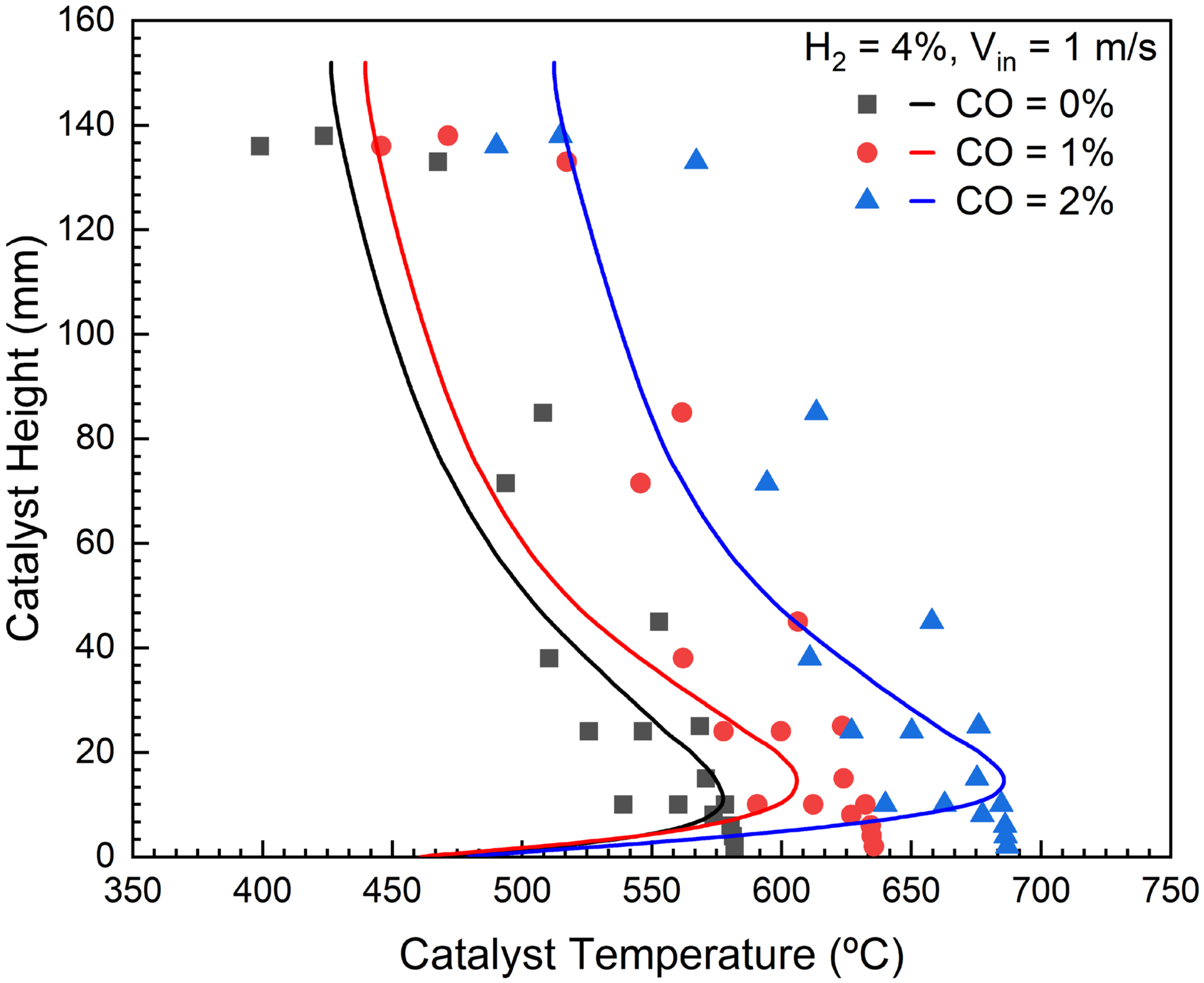




- Plate base: higher temperatures
  - Higher H_2 concentrations
- Plate top: lower temperatures
  - Lower H_2 concentrations
  - Heat losses
- Model reproduces well experimental data

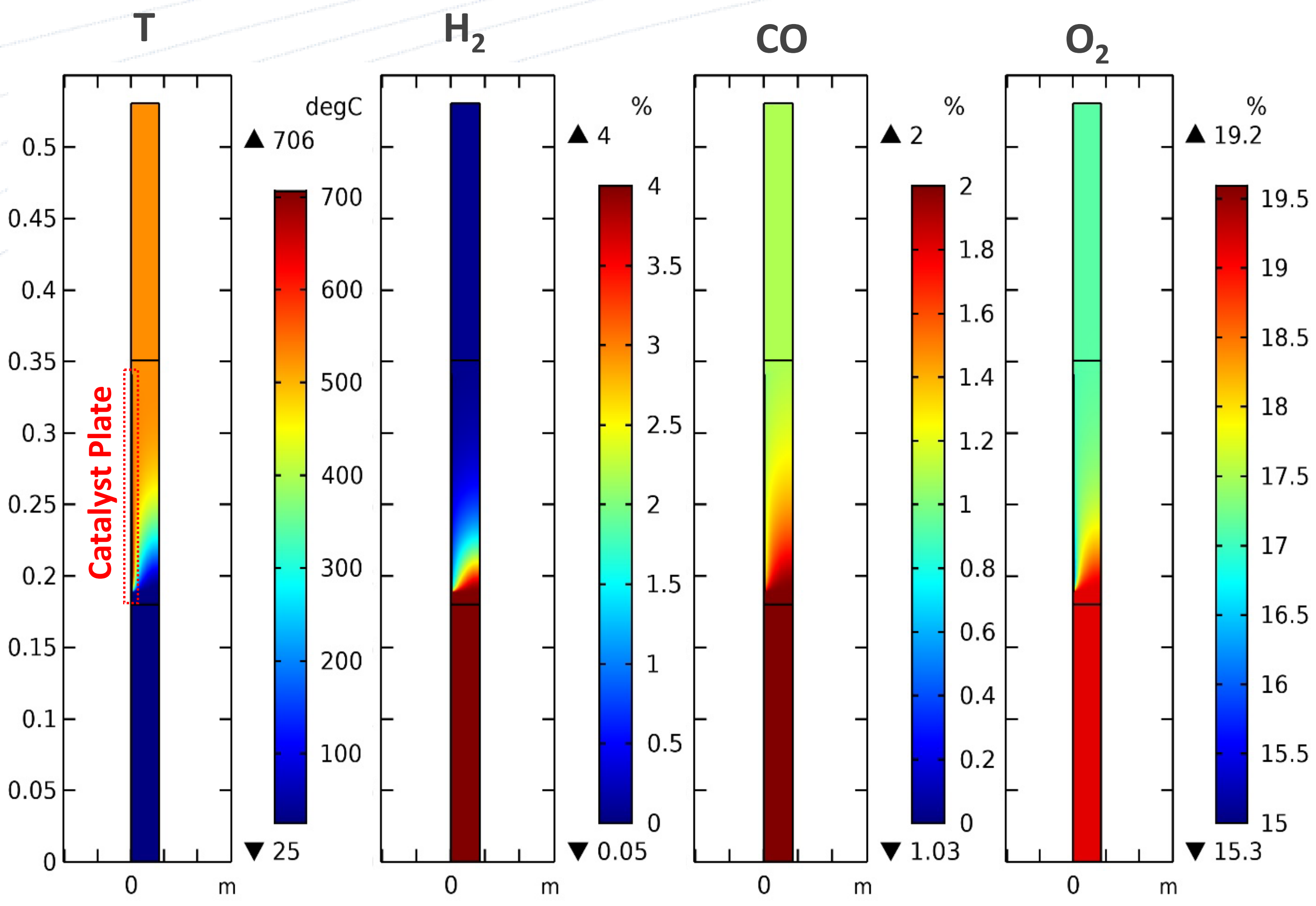
2D Transient PAR Model: Validation





- Plate base: higher temperatures
  - Higher H_2 concentrations
- Plate top: lower temperatures
  - Lower H_2 concentrations
  - Heat losses
- Model reproduces well experimental data
- Model reproduces well experiments at different conditions

2D Transient PAR Model: Contour Profiles ($H_{2,in}$=4%, V_{in}=1 m/s, CO_{in}=2%)



- **Temperatures:** Higher at the catalyst plate, lower at the channel.
- **H_2:** Entirely recombined.
- **CO:** Not entirely recombined.
- **O_2:** in excess (no O_2 limitations)

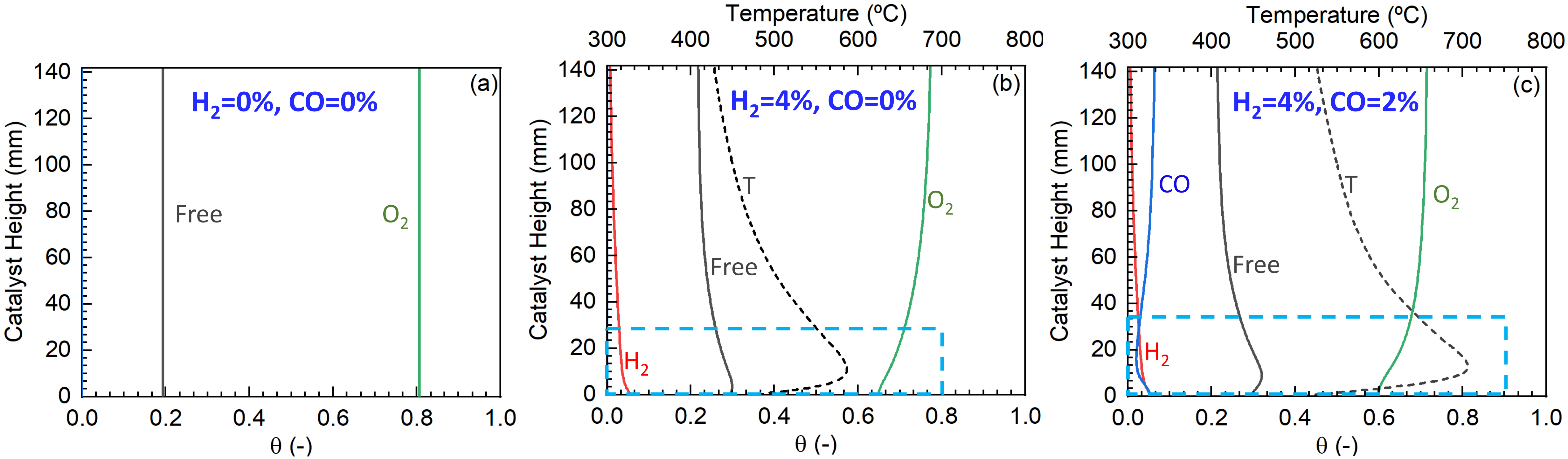
2D Transient PAR Model: Catalyst Surface Properties

$$\theta_i = \frac{\sigma_i c_{s,i}}{\Gamma_s}$$

θ_i= Fractional surface coverages.
Γ_s= density of sites of the surface.
σ_i= site occupancy number.
$c_{s,i}$= surface concentrations.

$$\theta_{free} = 1 - \sum_i \theta_i$$

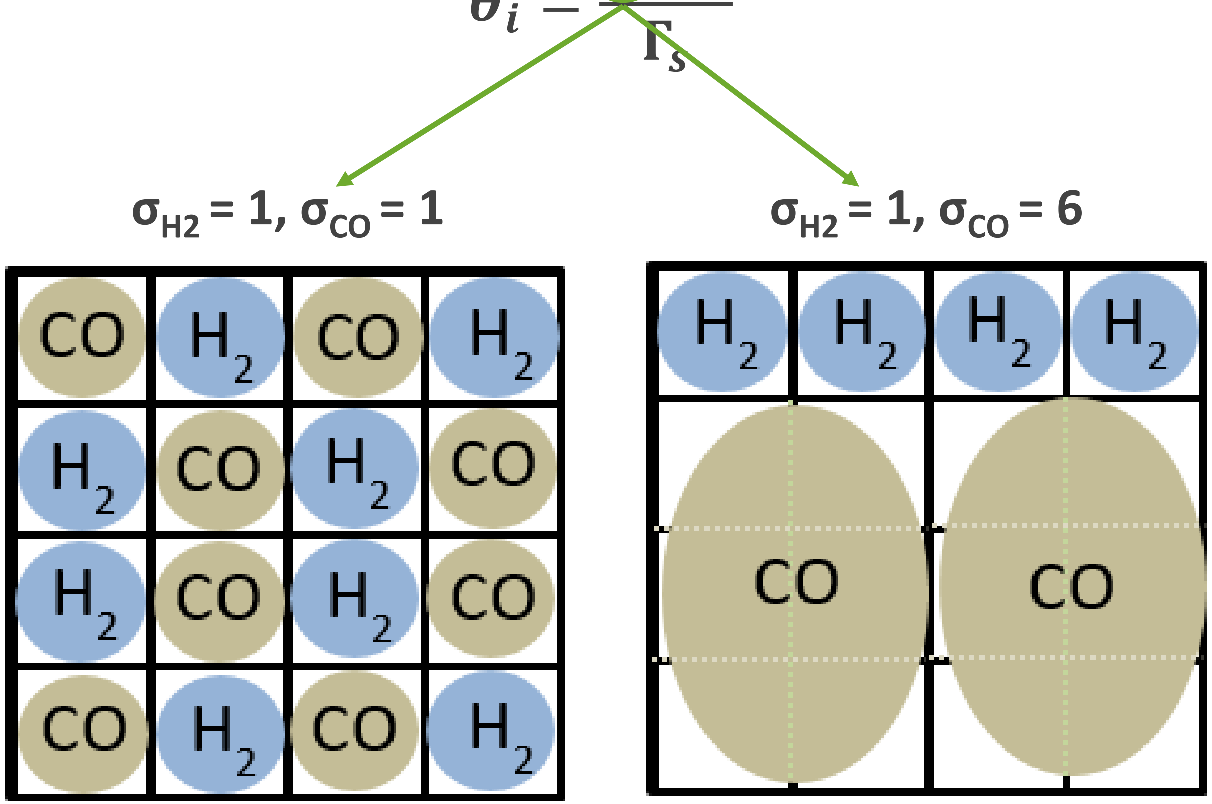
θ_{free}= fraction of free sites on the surface.



2D Transient PAR Model: Example of Poisoning

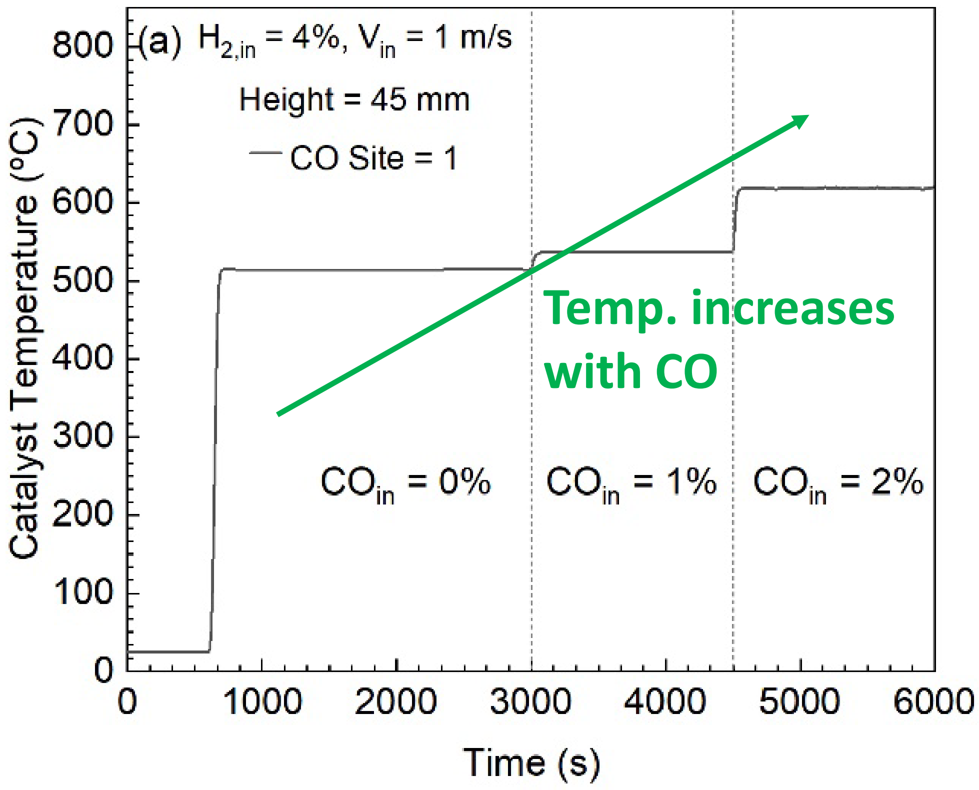
- CO Poisoning (Note: CO was only used as an example!! In reality, this might be different)
- Site occupancy number (σ) was manually increased

$$\theta_i = \frac{\sigma_i c_{s,i}}{\Gamma_s}$$

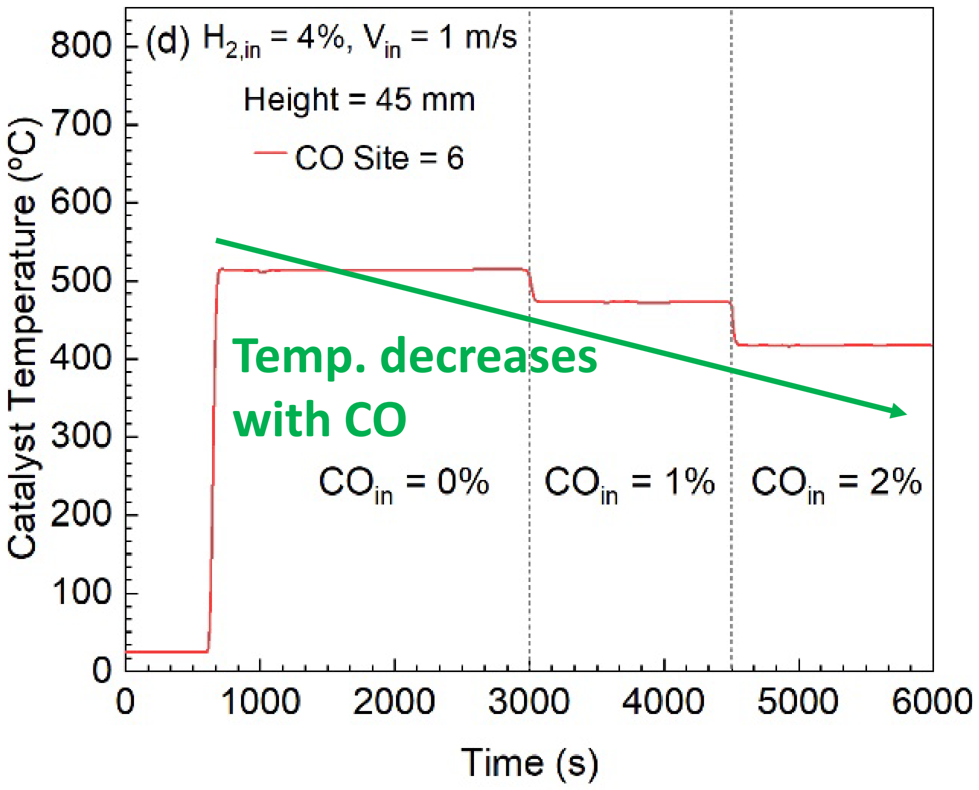


2D Transient PAR Model: Example of Poisoning

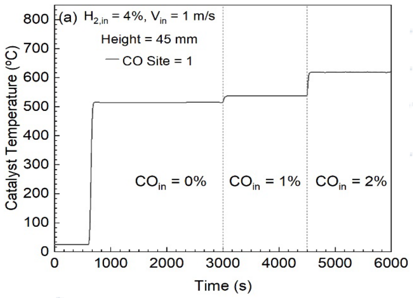
$\sigma_{H2} = 1, \sigma_{CO} = 1$



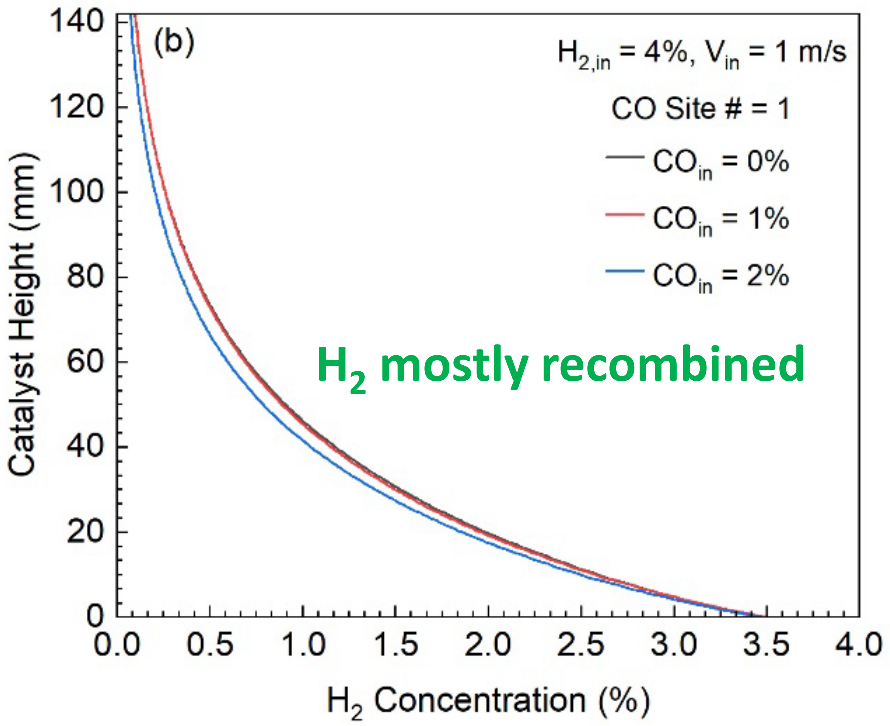
$\sigma_{H2} = 1, \sigma_{CO} = 6$



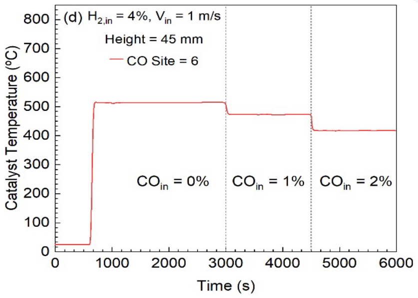
2D Transient PAR Model: Example of Poisoning

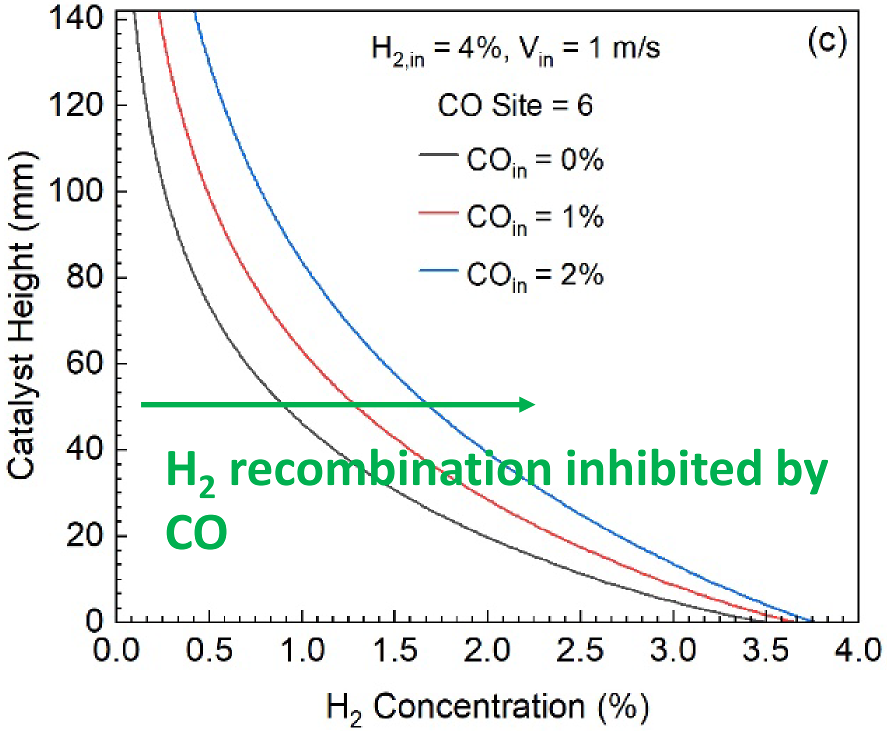


$\sigma_{H2} = 1, \sigma_{CO} = 1$



$\sigma_{H2} = 1, \sigma_{CO} = 6$





Summary

- H_2 and CO recombination reactions were tested in a 2D transient CFD model to simulate PAR performance.
- The model matched experimental catalyst temperature well along different conditions.
- Surface properties were simulated as a new feature in the model.
- Catalyst poisoning was tested showing that the model can handle such scenarios.
- Altogether, the model shows how surface chemistry can be used as tool to explain interesting mechanisms that cannot be easily seen in experiments.

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Questions?

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