

Computational particle fluid dynamics 3D simulation of the sorption-enhanced steam methane reforming process in a dual fluidized bed

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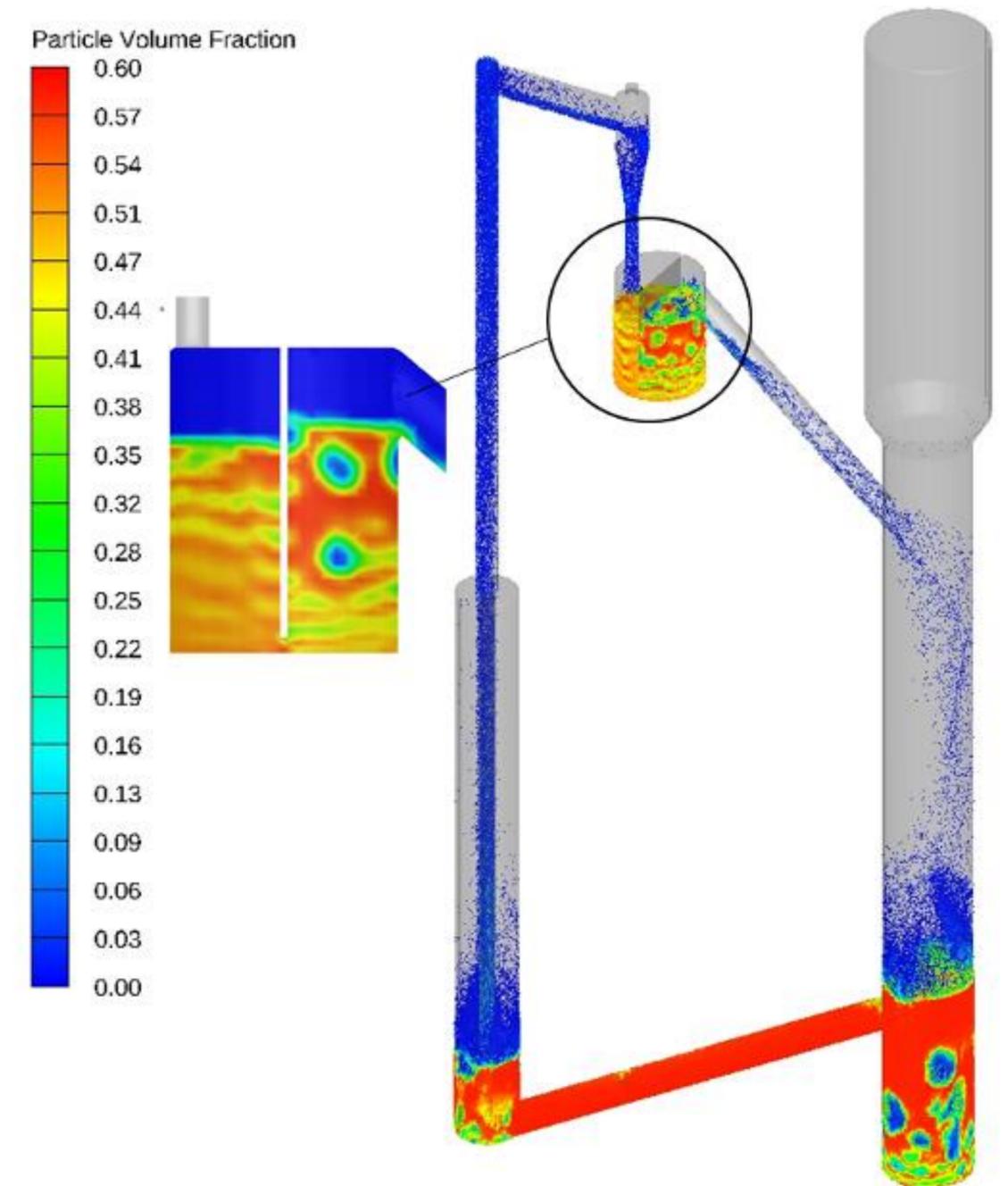
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Federico Monterosso (presenter), OMIQ Srl, Italy

Agenda

- A few words about ENEA and OMIQ
- Introduction to the project
- Dual Fluidised Bed Description
- Barracuda Virtual Reactor Model (Fluid and Chemistry setup)
- Lab Scale Reactor Model Validation
- Results
- Conclusions



A couple of words about ENEA and OMIQ



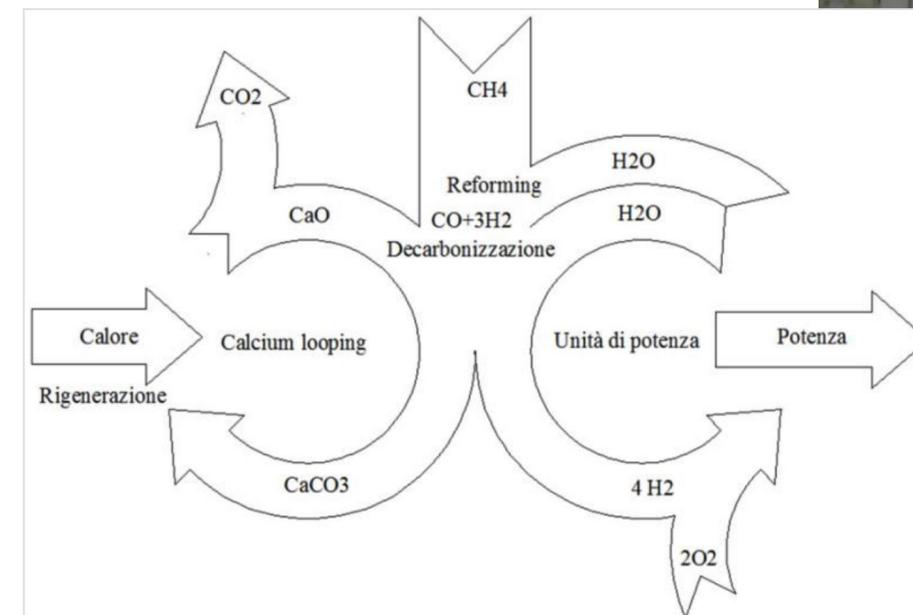
- ENEA is the Italian Agency for New Technologies, Energy and Sustainable Economic Development, a public body aimed at research, technological innovation and the provision of advanced services to enterprises, public administration and citizens in the sectors of energy, the environment and sustainable economic development.
- OMIQ srl is the Barracuda Virtual Reactor distributor for Italy. A software engineering company focused on vertical simulation solutions founded by two Italian engineers with a passion for simulation and design. Our mission is to provide help to companies focused on innovation, looking to improve their design process and optimise their products.



Project Background

ZECOMIX (Zero Emission of CarbOn with MIXed Technologies)

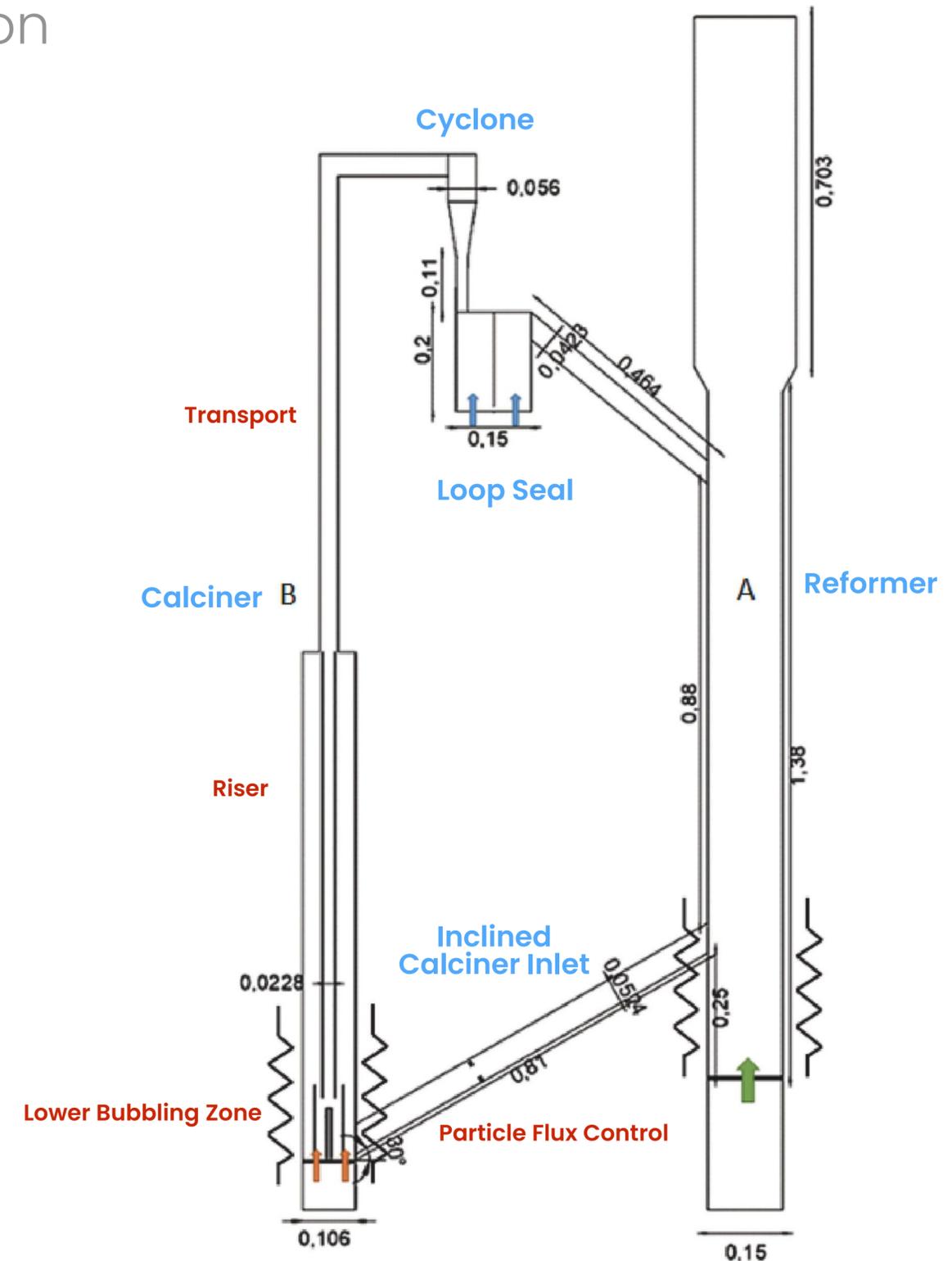
- Zecomix Pilot Plant
- Dual Fluidised bed -> Continuous Process
 - Reformer
 - Calciner -> Sorbent Regeneration
- H2 Production + CO2 Capture
 - Bifunctional Particles -> Sorbent Catalyst



The Dual Fluidised Bed

Description

- Bubbling Reformer ($T = 650^{\circ}\text{C}$)
- Partially Bubbling Calciner Reactor ($T = 950^{\circ}\text{C}$)
- Cyclone: CO_2 gas - regenerated particles separation
- Loop Seal: allows particles flow/avoid gas flow
- Inclined Calciner Inlet
- Reformer Thermal Input: 1.87 KW
- Calciner Thermal Input: 3.82 KW



Barracuda Virtual Reactor Model

Fluid Dynamics

- Mesh: 1.1 million cells , including refinement
- EMMS Drag Model: capable to capture the heterogeneous structures in the overall system
- Bifunctional Particles:
 - 60% CaO
 - 10% Ni
 - 30% Inert Support
 - D = 500 micron
- Inlet conditions
 - Reformer Fluidisation Gas mixture: Steam + Methane
 - H₂O/CO₂ Ratio = 3
 - Superficial Velocity = 2.5*U_{mf}
 - Calciner Fluidisation Gas : CO₂
 - Loop Seal Inlet Gas: Steam

Input data for reformer, calciner and loop seal.

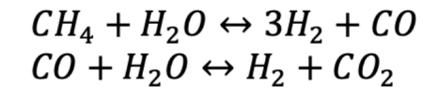
Reformer	
Fluidization gas flow	1.114·10 ⁻³ kg/s
Fluidization gas temperature	450 °C
Fluidization gas composition (%mol)	25% CH ₄ 75% H ₂ O
Wall heat power input	1.87 kW
Hold up	4.6 kg
Calciner	
Fluidization gas flow	1.169·10 ⁻³ kg/s
Fluidization gas temperature	450 °C
Fluidization gas composition	CO ₂
Nozzle gas flow	1.25·10 ⁻³ kg/s
Nozzle gas input temperature	574 °C
Nozzle gas composition	CO ₂
Wall heat power input	3.82 kW
Hold up	1 kg
Loop seal	
Recycle chamber gas flow	2.131·10 ⁻⁴ kg/s
Supply chamber gas flow	1.421·10 ⁻⁴ kg/s
Gas input Temperature	450 °C
Gas composition	H ₂ O

Barracuda Virtual Reactor Model

Chemistry

- Thermal Radiation on
- Chemistry
 - Sorption Enhanced Steam Methane Reforming
 - ▶ CO₂ sorption modelling: shrinking core approach
 - Calcination Reaction
 - ▶ TGA Experimental Data Fit + Fang et.al.

SE-SMR scheme by Numaguchi-Kikuchi



$$r_{SMR} = \frac{k_{SMR}^0 \cdot e^{\left(\frac{-E_{SMR}}{RT}\right)} \cdot \left(P_{CH_4} \cdot P_{H_2O} - \frac{P_{CO} P_{H_2}^3}{K_{eq,SMR}} \right)}{P_{H_2O}^{1.596}}$$

$$r_{WGS} = \frac{k_{WGS}^0 \cdot e^{\left(\frac{-E_{WGS}}{RT}\right)} \cdot \left(P_{CO} \cdot P_{H_2O} - \frac{P_{CO_2} P_{H_2}}{K_{eq,WGS}} \right)}{P_{H_2O}}$$

CO₂ sorption rate by Stendardo-Foscolo

$$r_s = \frac{N_{CaO}^0 \cdot \sigma_{CaO}^0 \cdot k_{CBN} (1 - X_{CaO})^{2/3} (C_{CO_2} - C_{CO_2,eq})}{1 + \frac{N_{CaO}^0 \cdot k_{CBN} \cdot \delta_{CaO}^0}{2D_{pl}} \sqrt[3]{1 - X_{CaO}} \left(1 - \sqrt[3]{\frac{1 - X_{CaO}}{1 - X_{CaO} + X_{CaO} \zeta}} \right)}$$

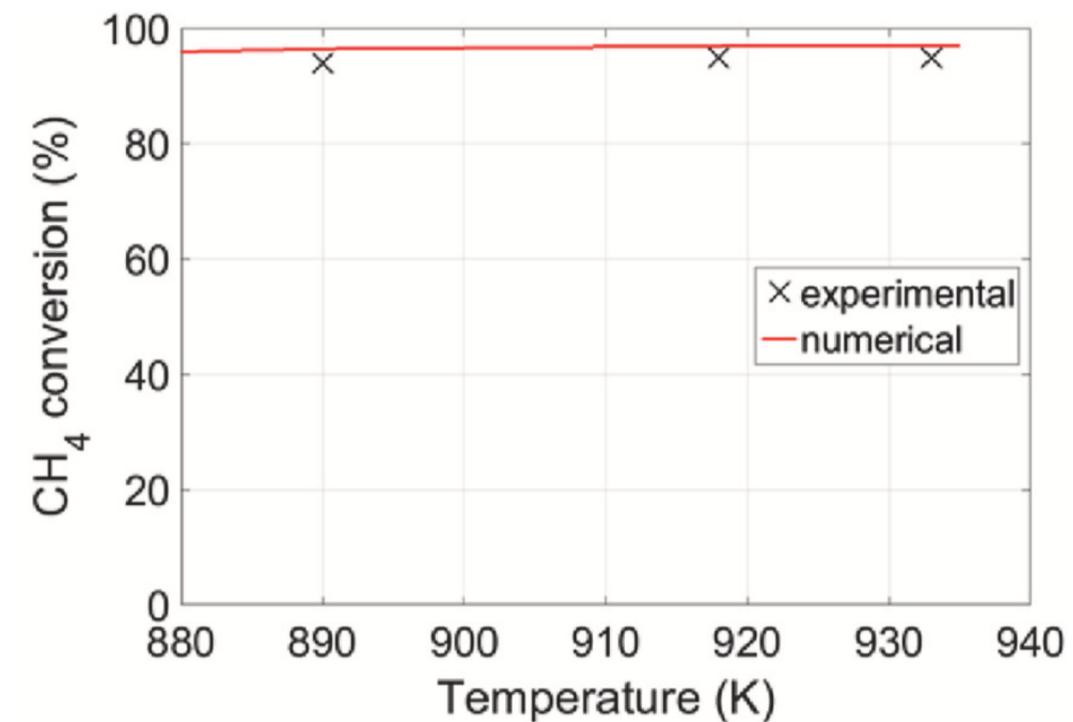
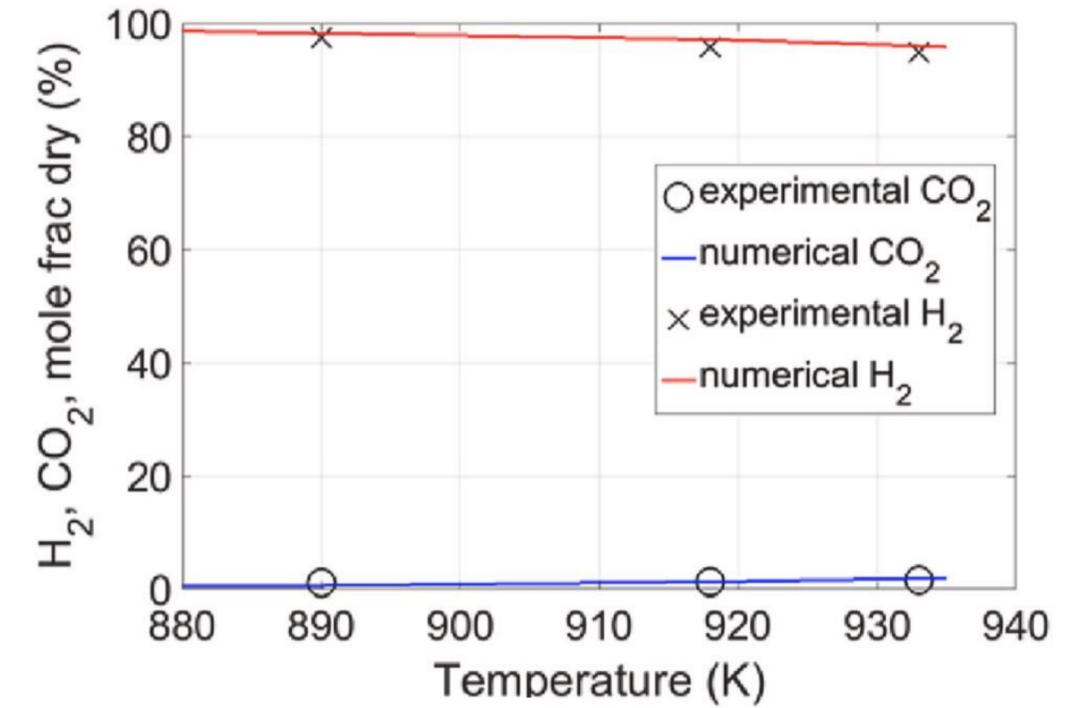
Calcination reaction scheme by Fang et al. + Exp Data fit



$$\frac{dX}{dt} = k_c (1 - X)^{\frac{2}{3}} (C_{CO_2,eq} - C_{CO_2})$$

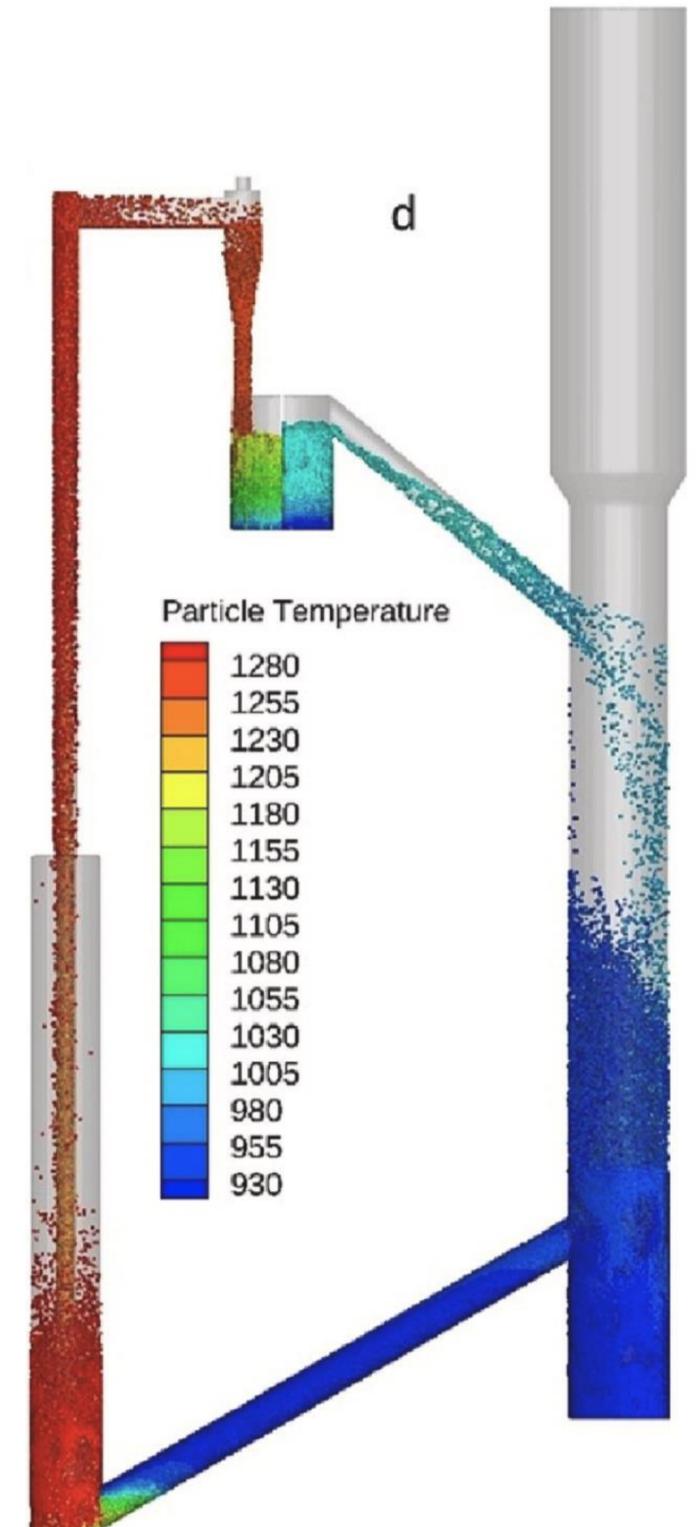
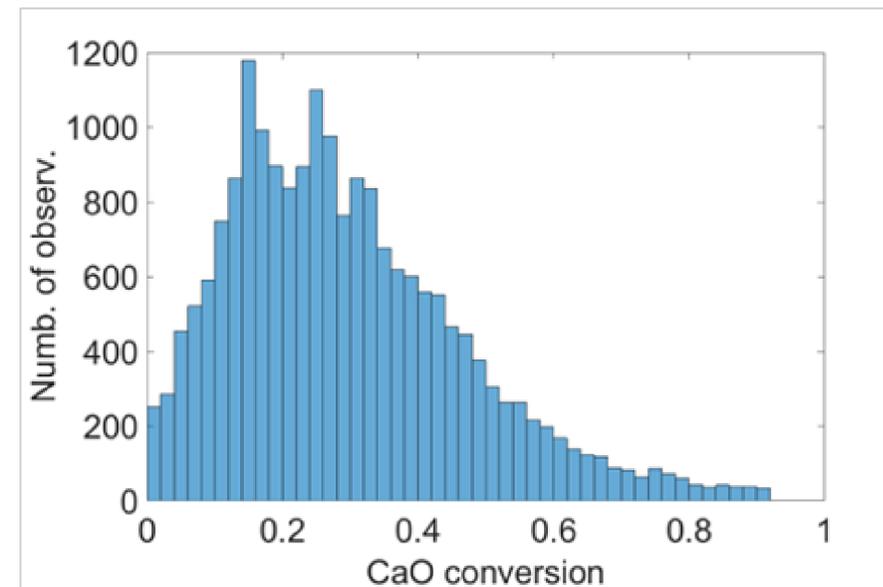
Lab-scale reactor validation

- Lab Scale reactor
 - Cylinder diameter: 8 cm
 - Bed height: 20 cm
- Calcined dolomite as sorbent
- Nickel-based catalyst
- Particles sizes were in the range 180–425 μm .
- Fluidization velocity: 0.15 m/s



Full vs Reduced Model

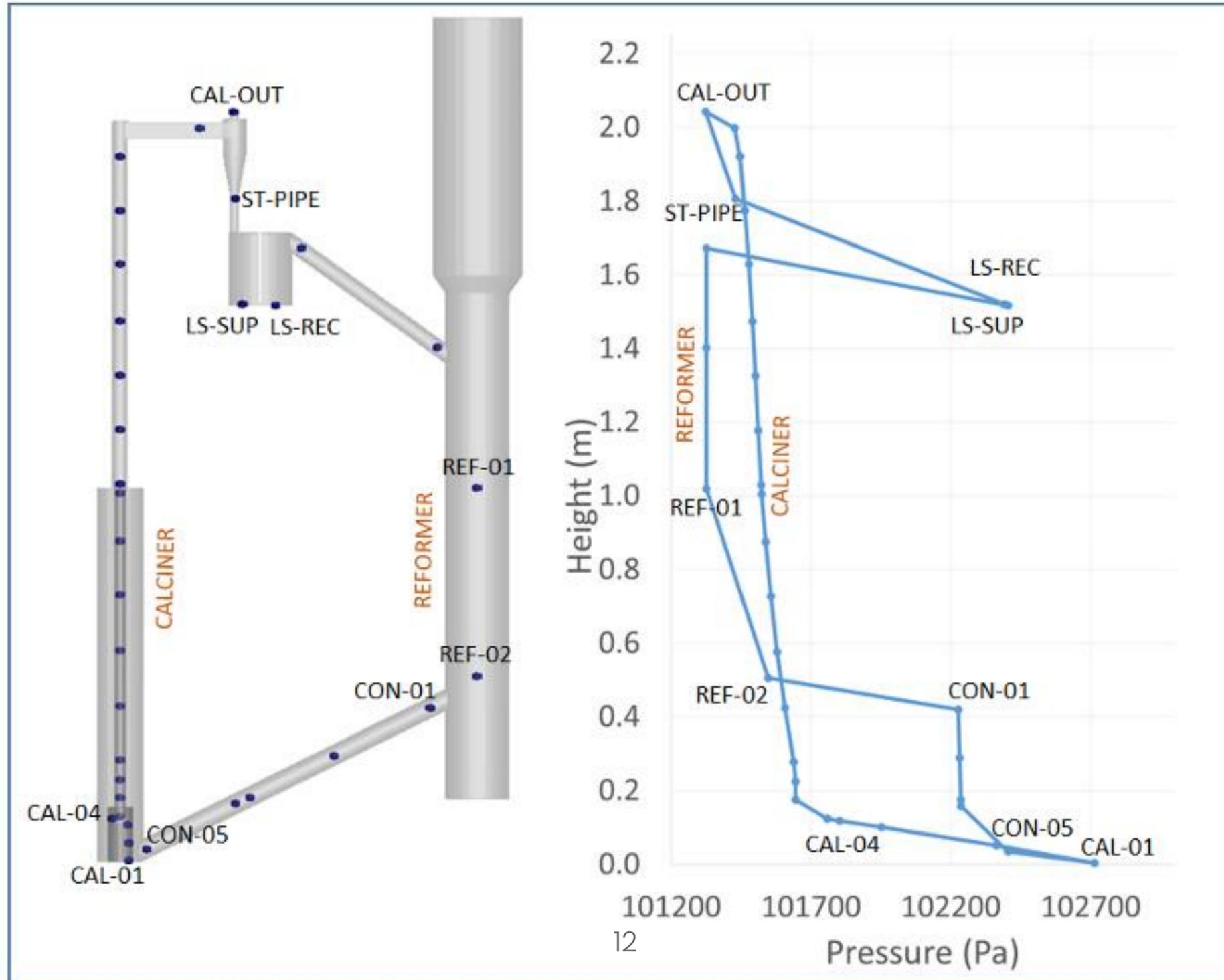
- The simulations were executed using a 2× Intel Xeon Platinum 8160 machine equipped with a GPU TESLA V100-PCIE-32GB.
- o(weeks) to achieve steady state behaviour
- Reformer-only model for particle composition initialization



Results Discussion

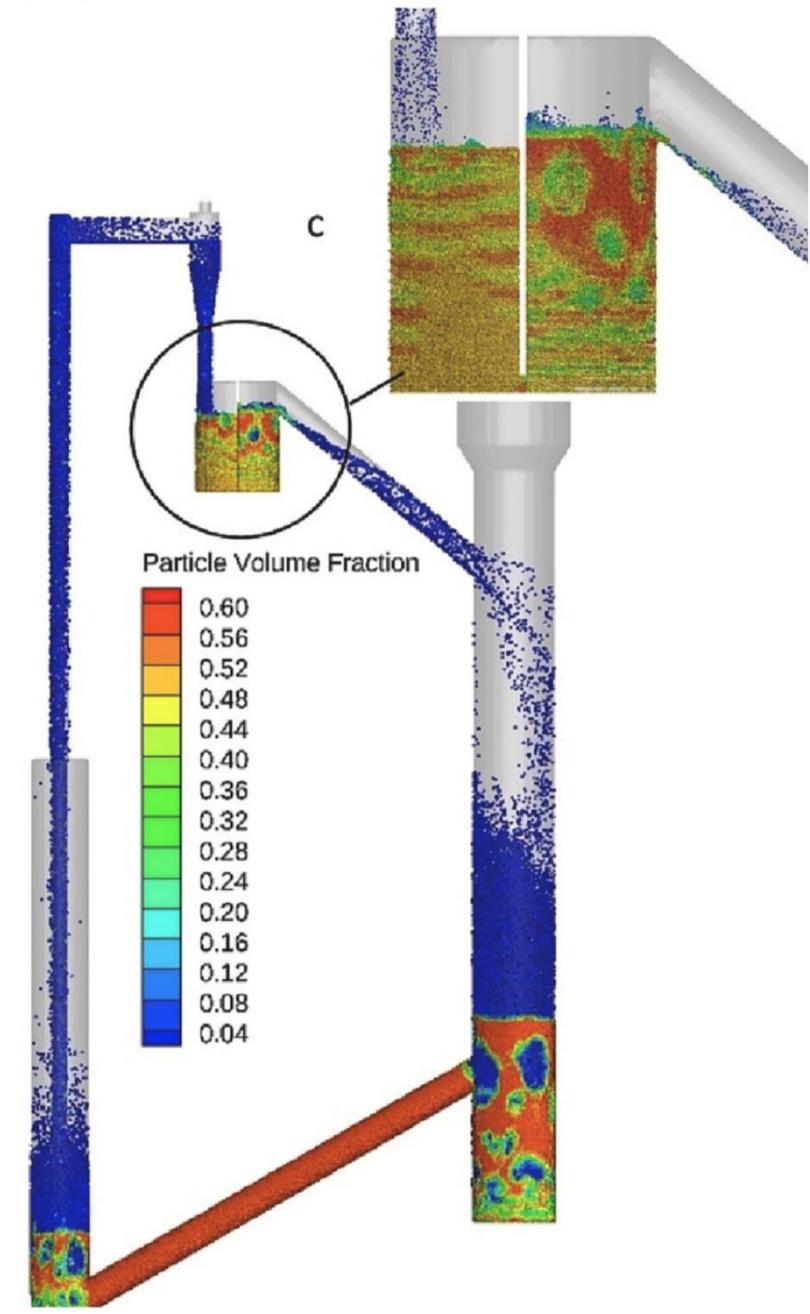
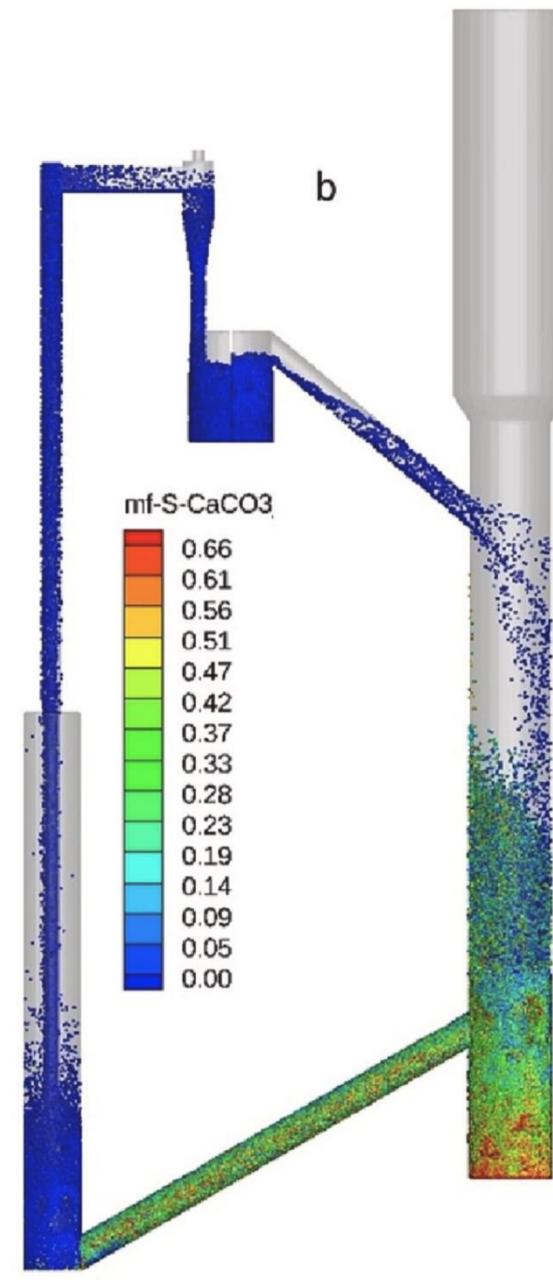
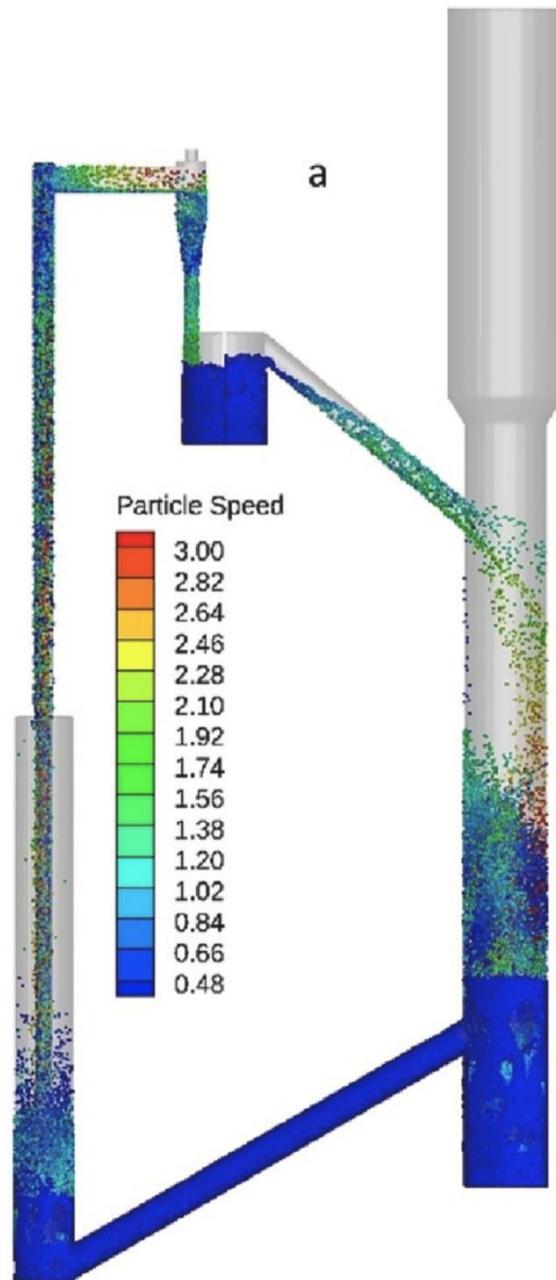
Full Model

Time-Averaged Pressure Profile across the system



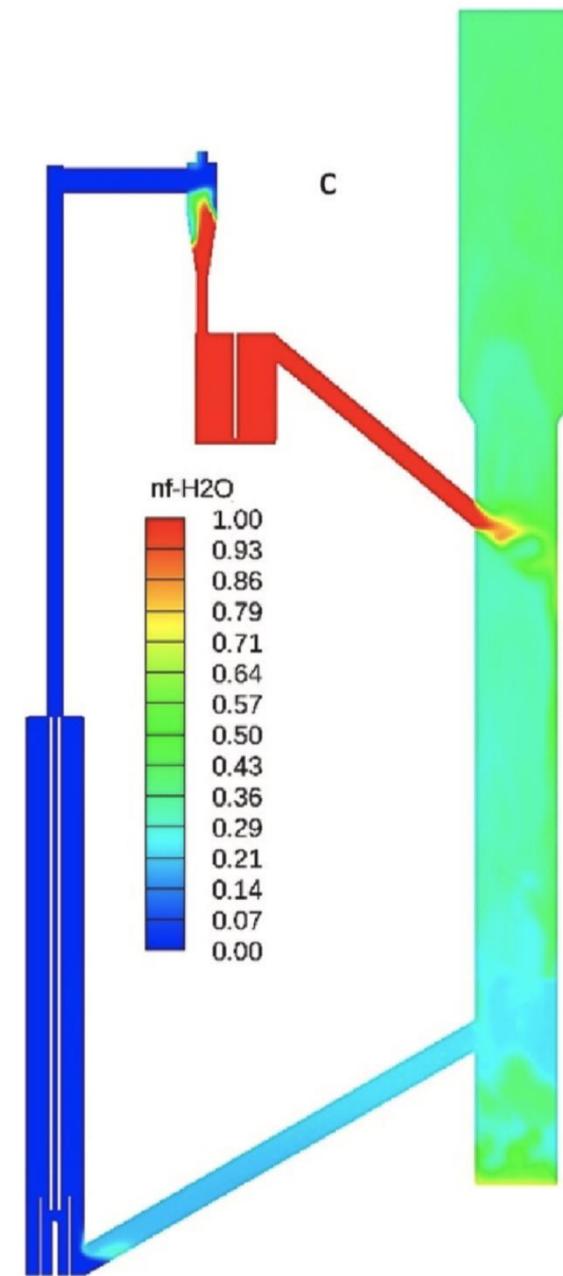
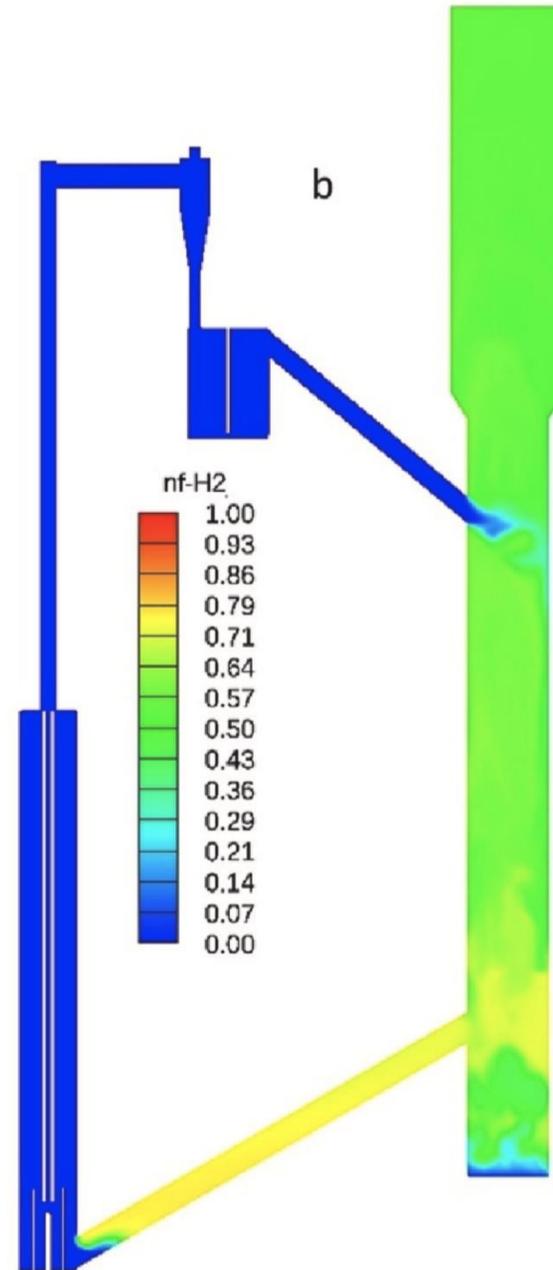
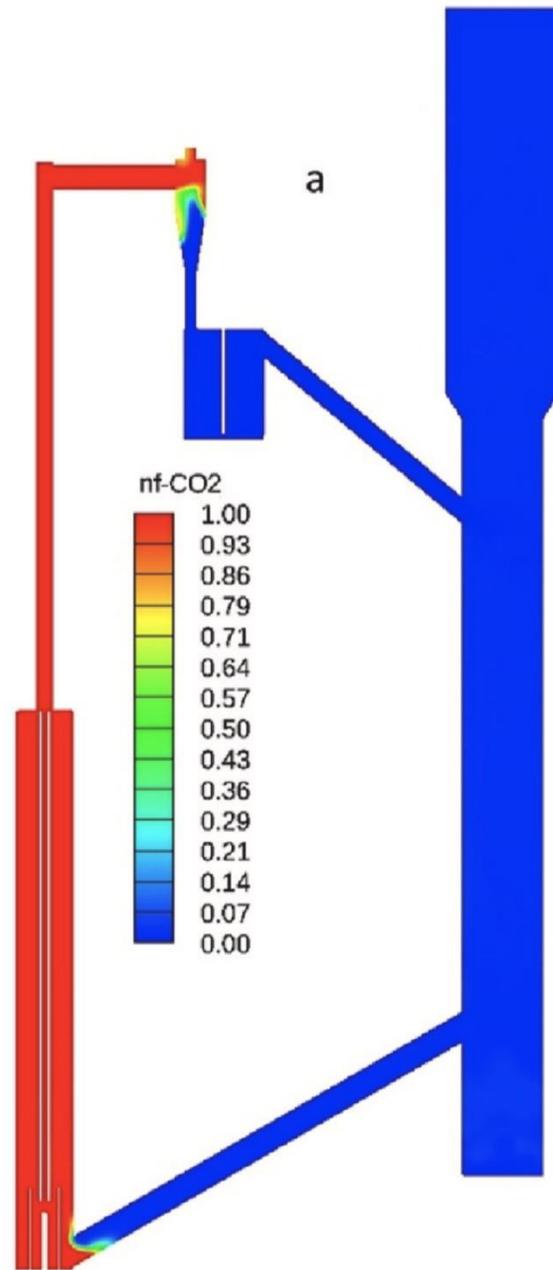
Full Model

Solids Across the System



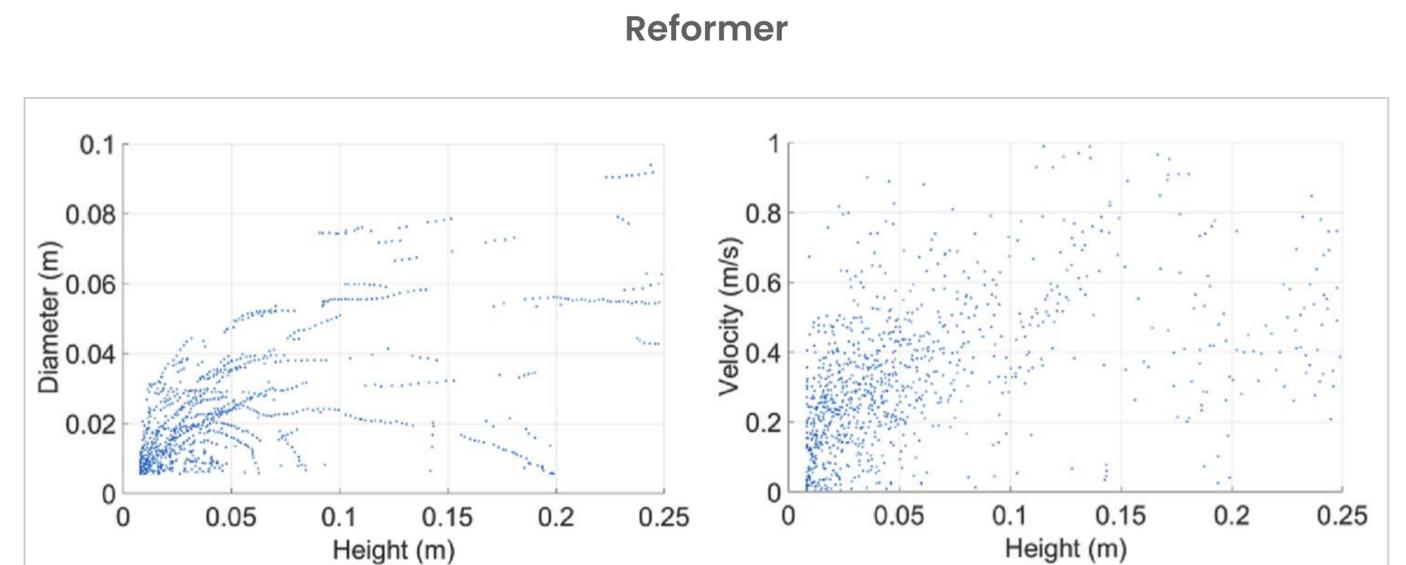
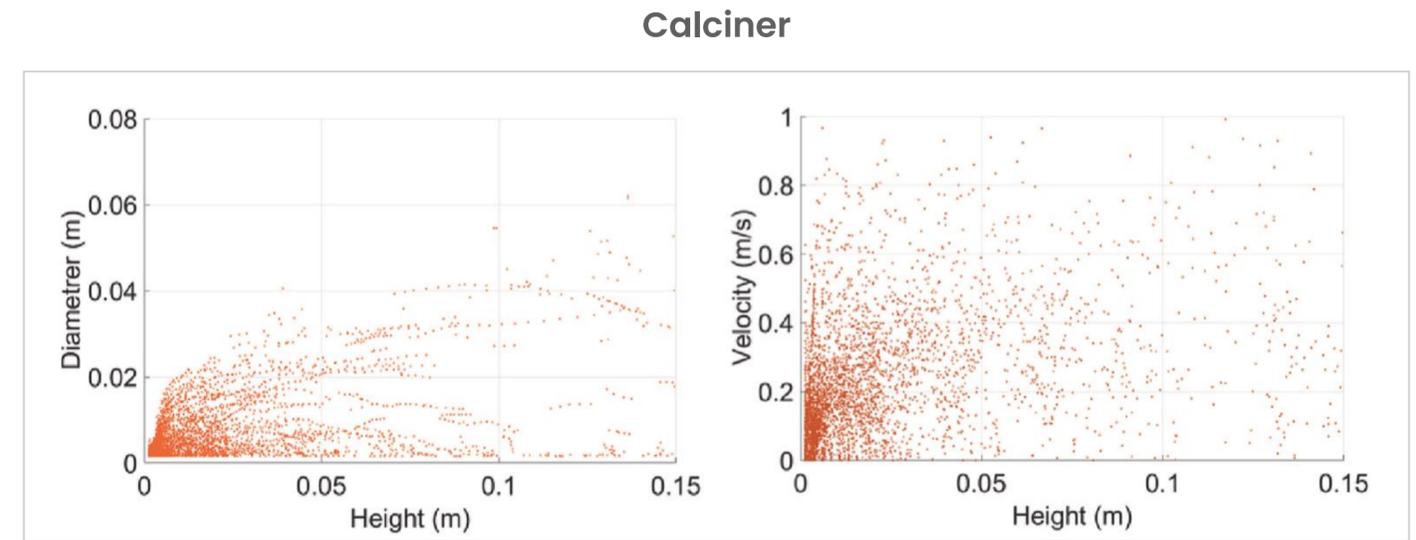
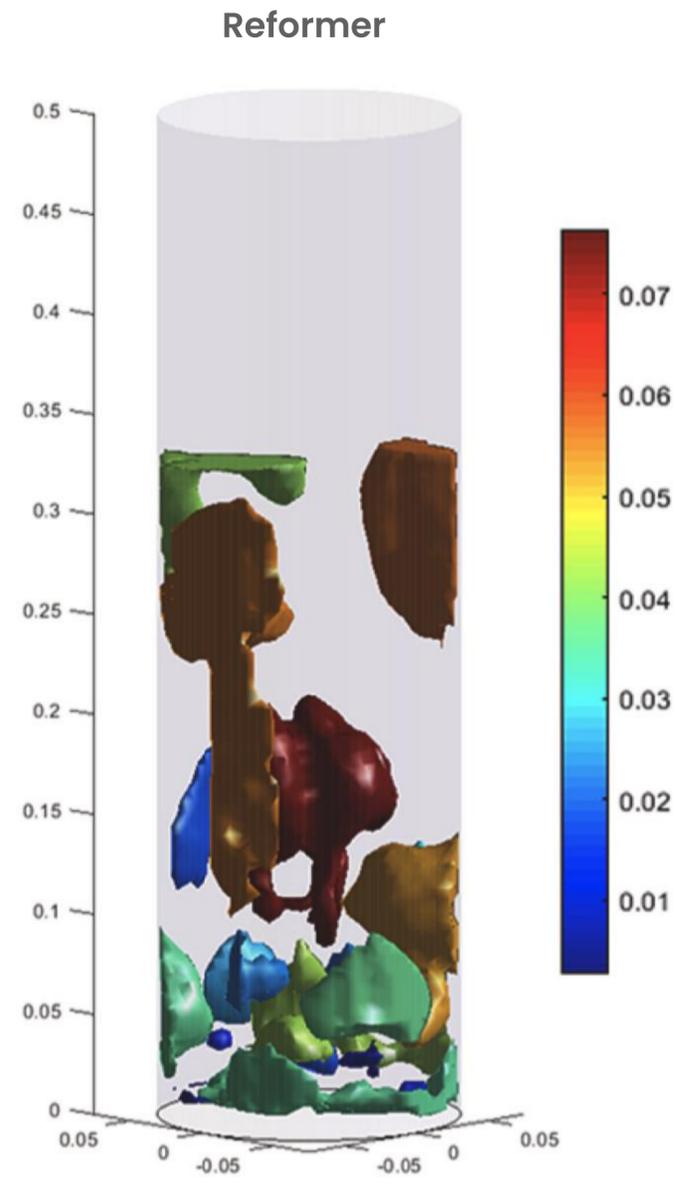
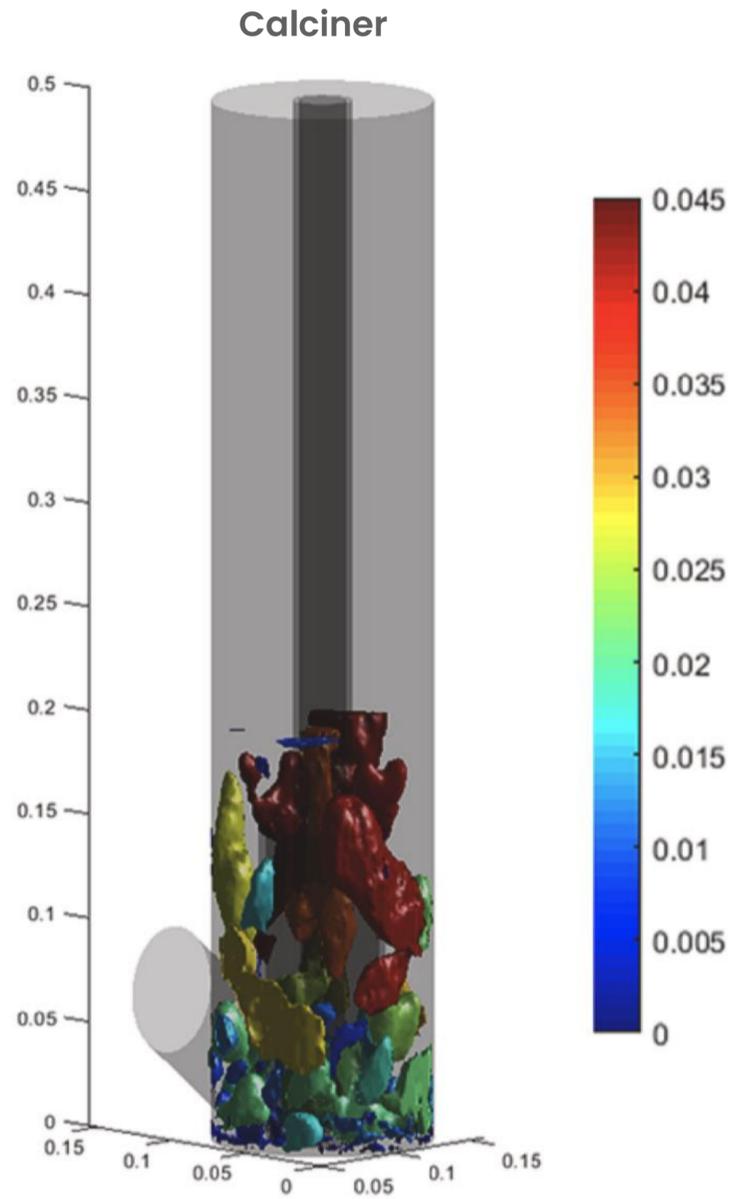
Full Model

Gas Fractions across the system



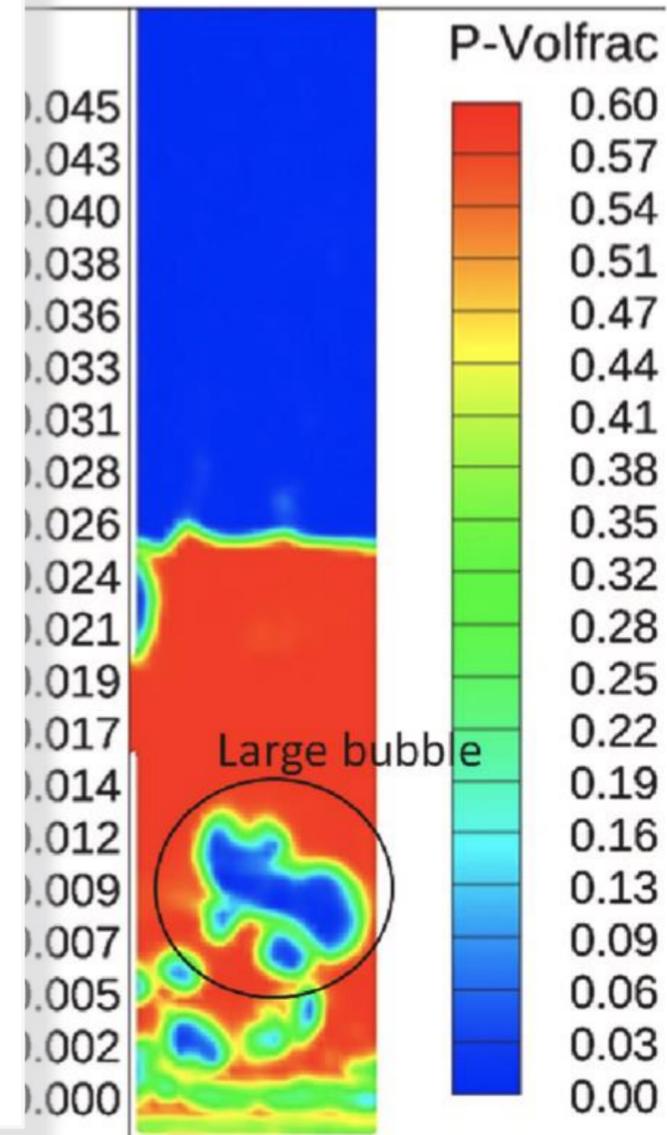
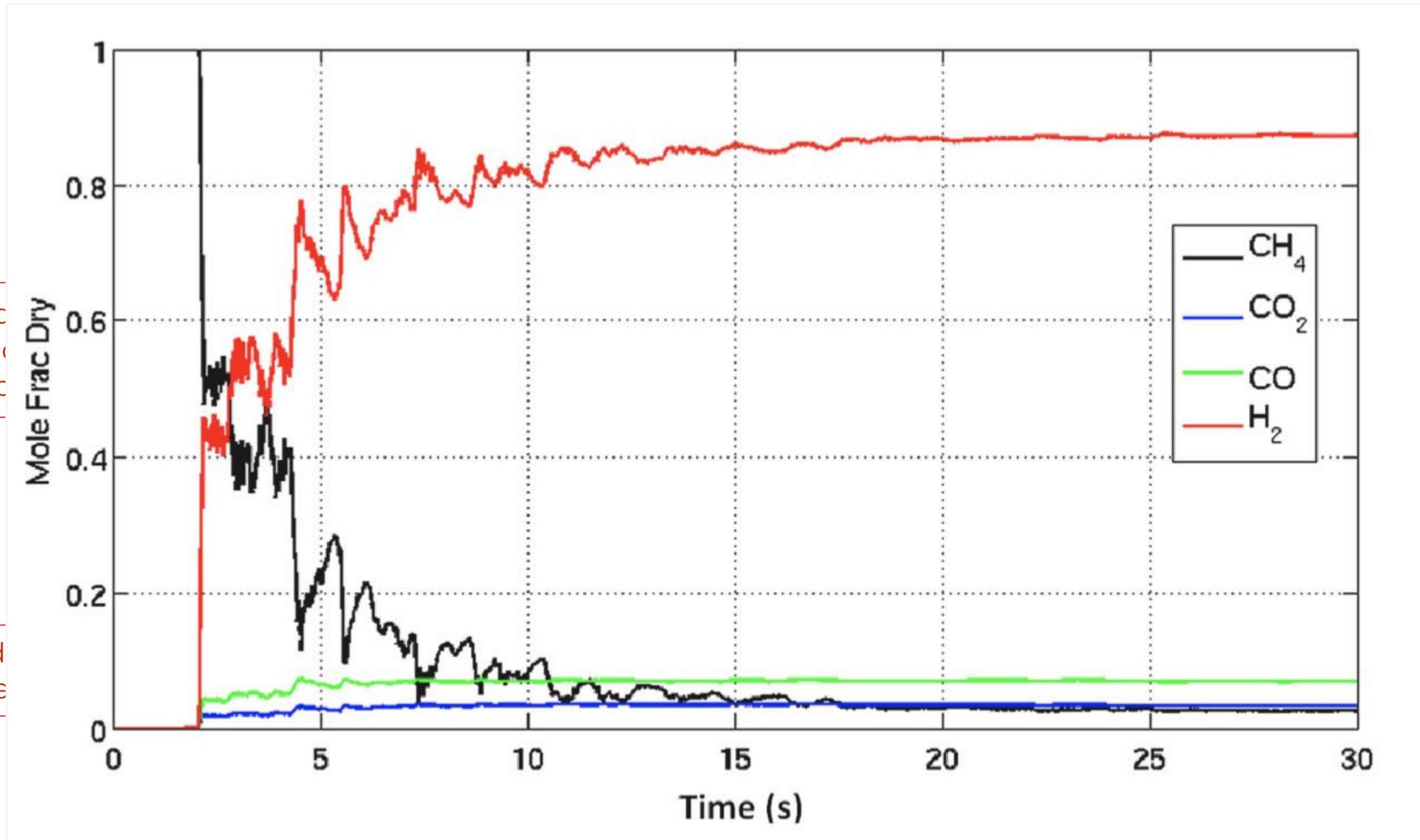
Full Model

Bubbles behaviour



Full Model

Bubbles behaviour and H2 Conversion

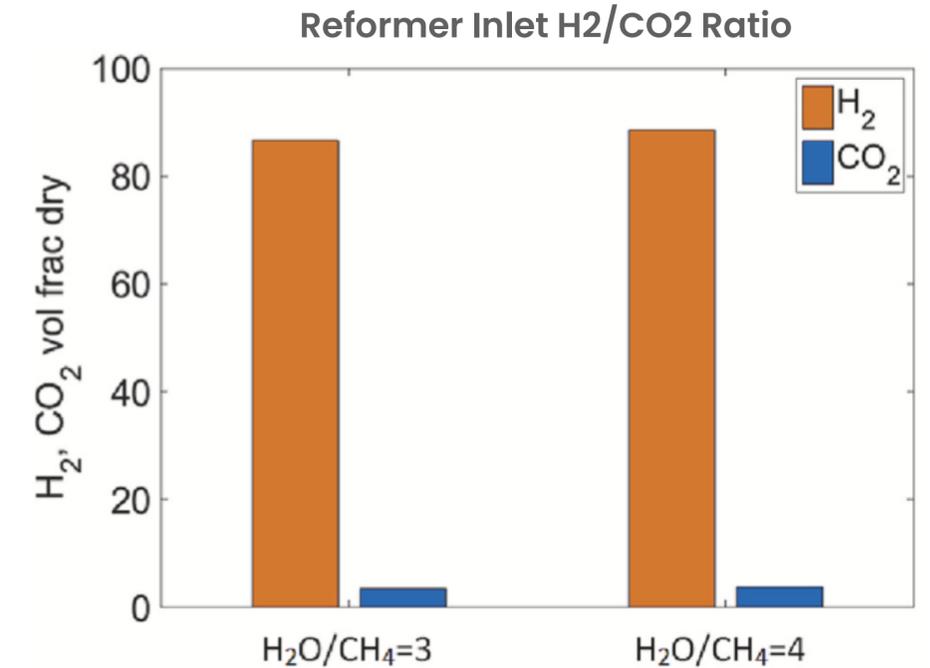
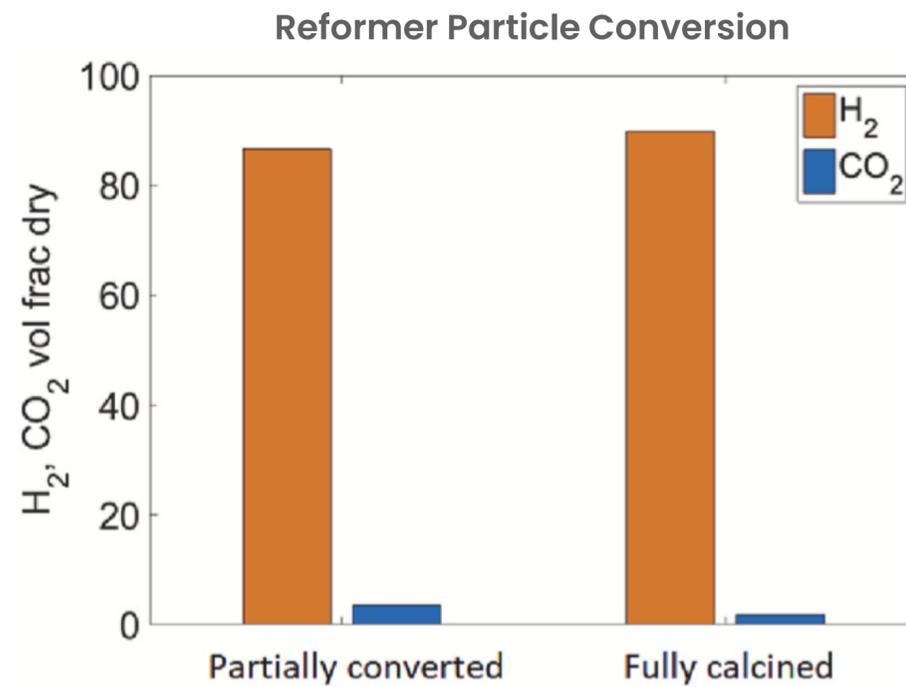
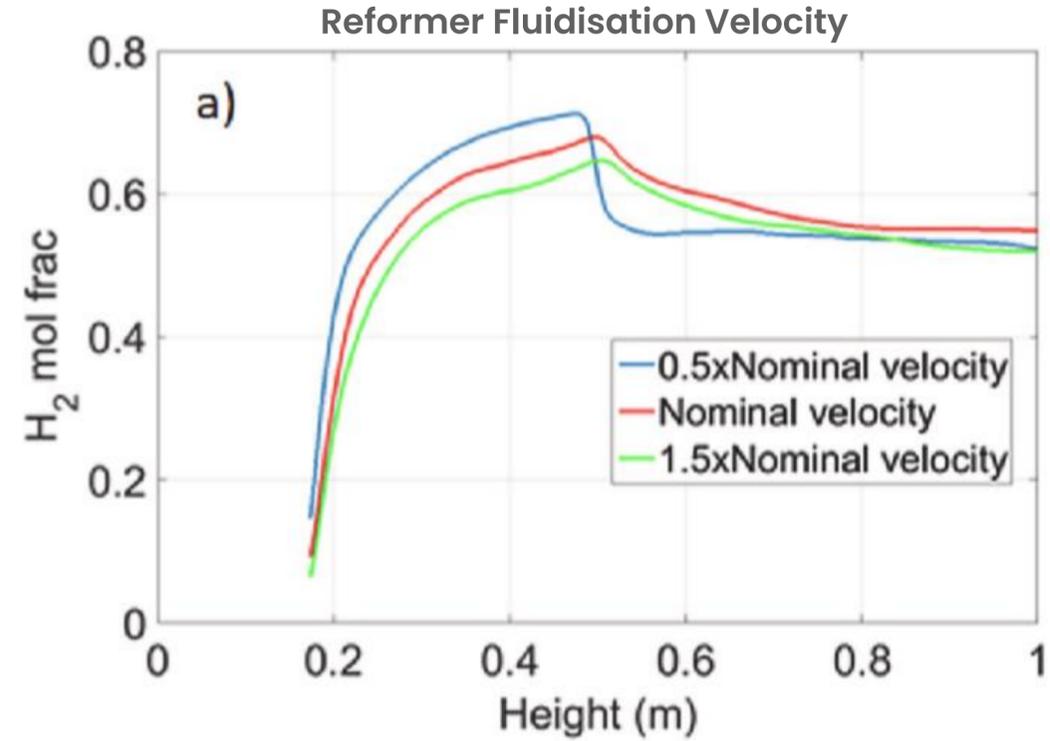
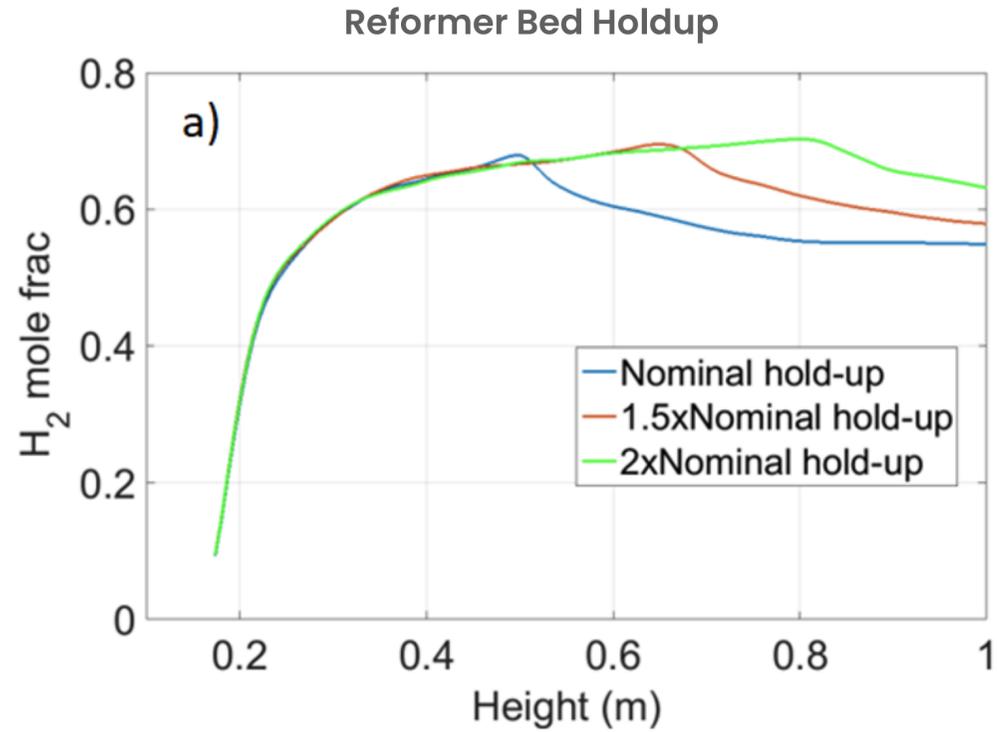


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Reformer-only Model

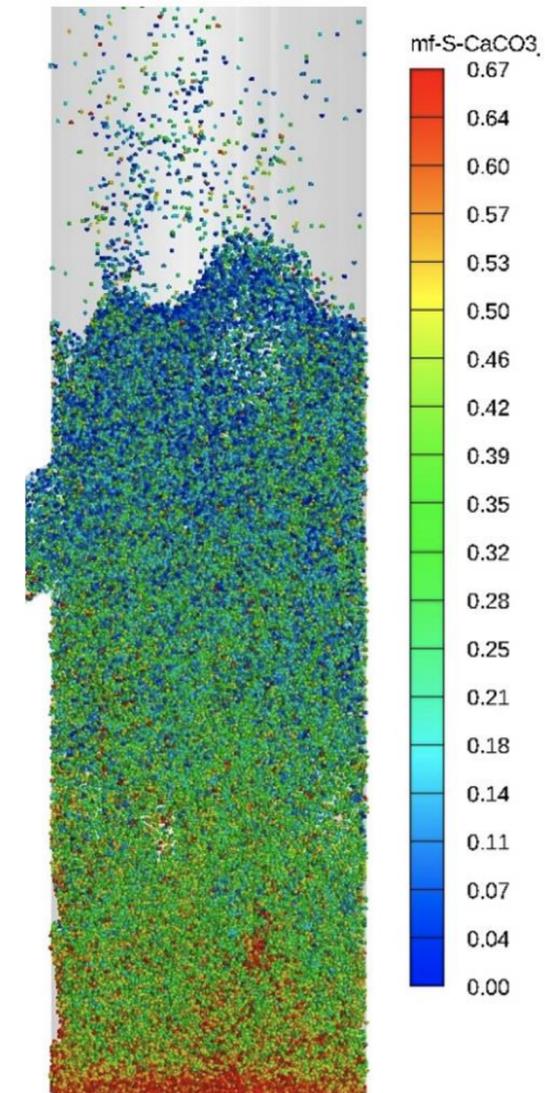
Reformer Operating Conditions



Conclusions

- A Dual Fluidized Bed has been studied with Barracuda Virtual Reactor
- The system combines steam methane reforming and carbon dioxide capture with exhausted particles regeneration in a single unit (continuous operation)
- Bifunctional particles based on Ni and CaO were used.
- Simulation results have been presented:
 - System Pressure profile
 - Solids and Gas Circulation features
 - Bubbles behaviour
 - Impact of operating conditions

- Barracuda Virtual Reactor proved to be a very efficient tool for the investigation of the behaviour of this type of systems



Conclusions

For further reference :

Powder Technology 424 (2023) 118568

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Questions ?





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