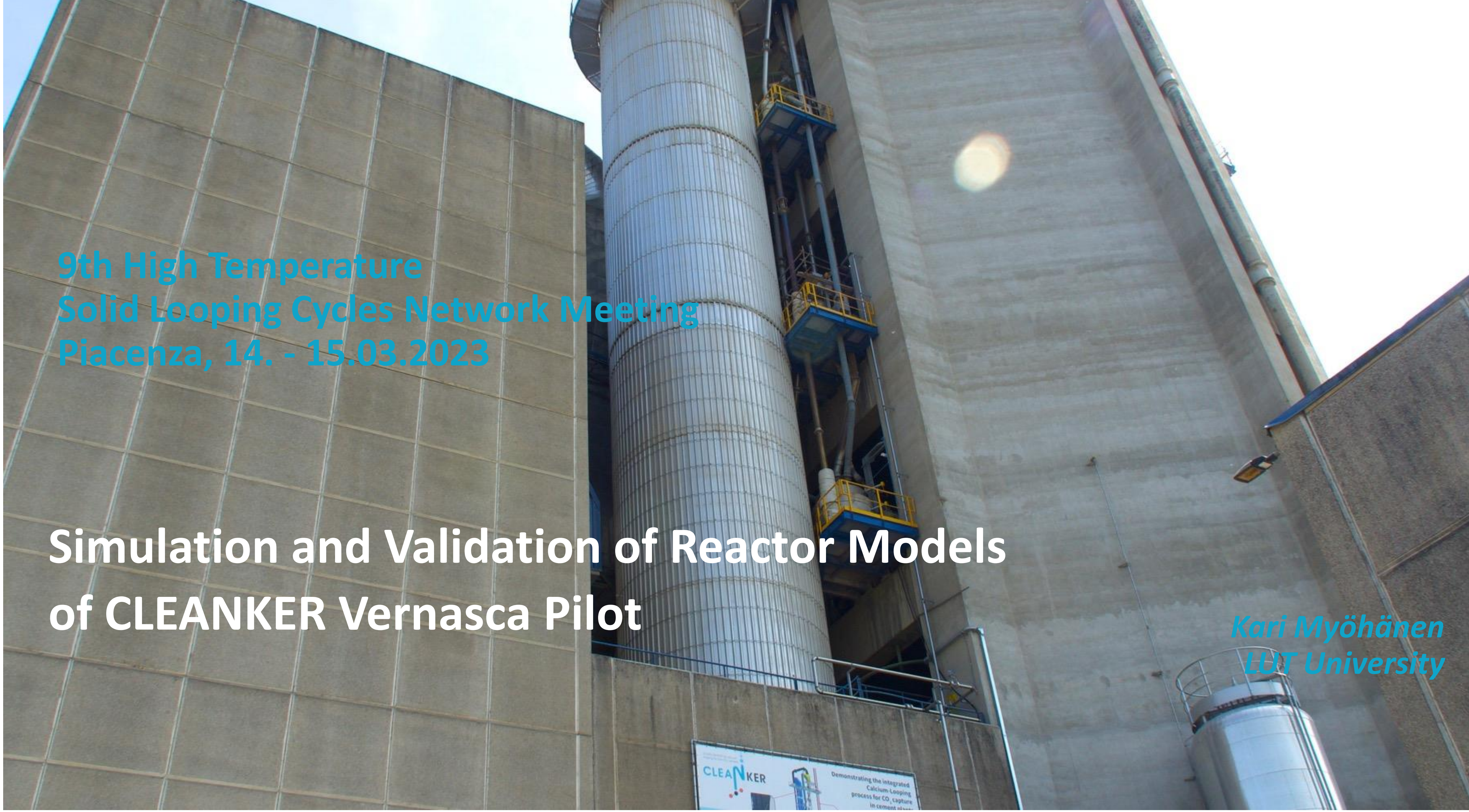

9th High Temperature
Solid Looping Cycles Network Meeting
Piacenza, 14. - 15.03.2023

Simulation and Validation of Reactor Models of CLEANKER Vernasca Pilot

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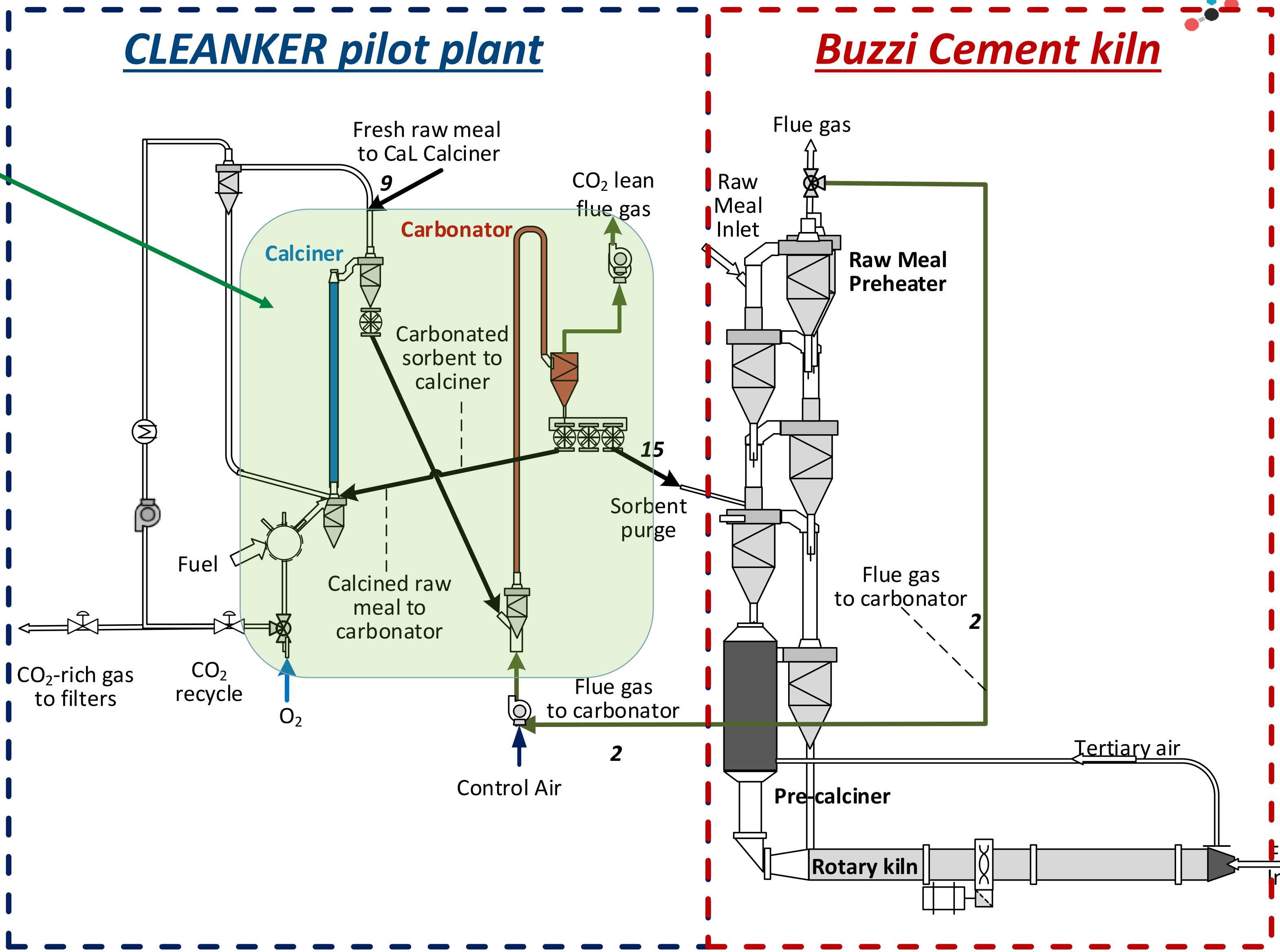
LUT University

Introduction

Scope of simulations: calciner and carbonator reactors

Contents of presentation

- Overview
- Global plant simulations
- 1D modelling
- 3D modelling
- Conclusions



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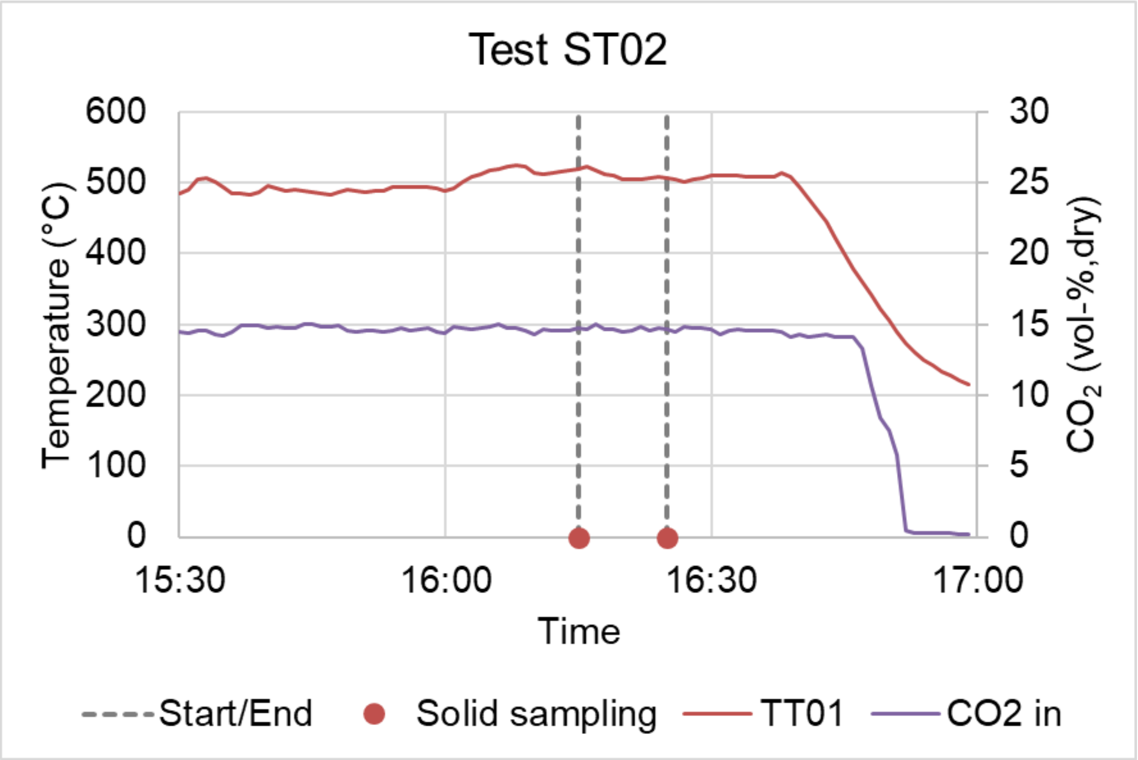
Overview: modeled pilot tests

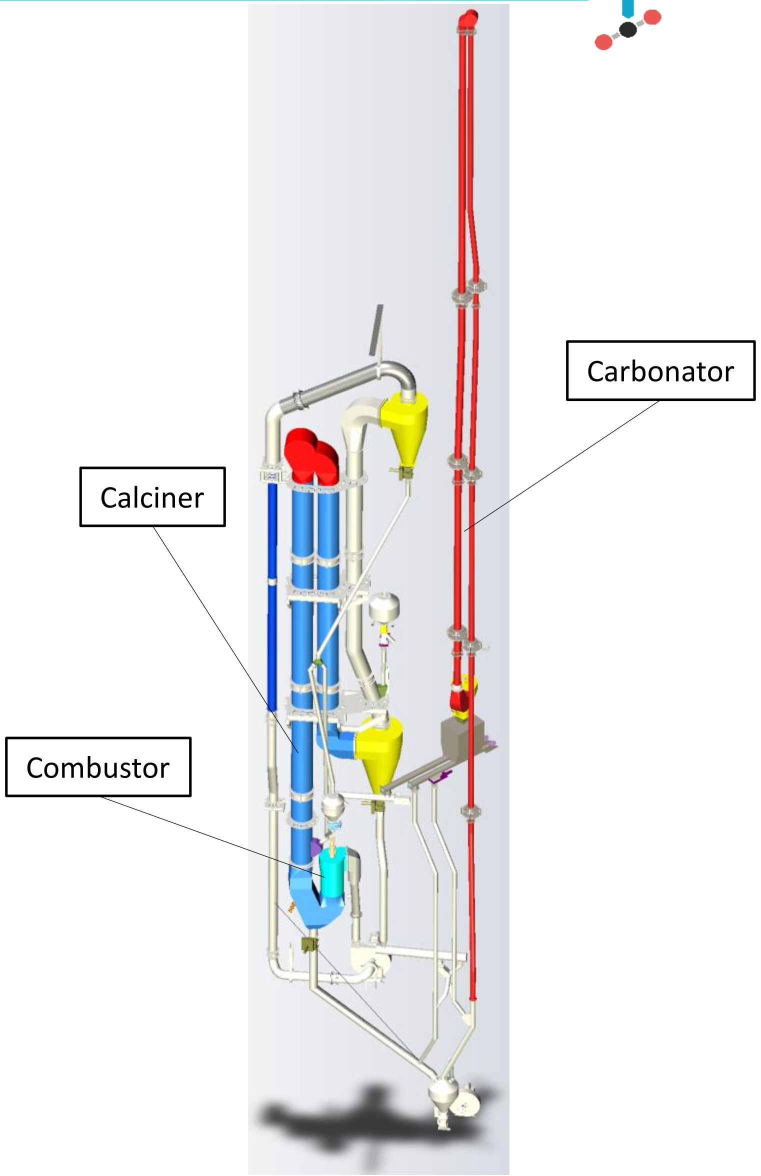
- Selected test balance times:
  - ST02: 29.4.2022 16:15 – 16:25
  - ST04a: 2.8.2022 11:33 – 11:45
  - ST04b: 2.8.2022 13:45 – 13:51
  - LT02: 1.12.2022 11:37 – 11:43

- The balance times were selected for intervals, in which solid samples were collected from calciner and carbonator.
- Actual test periods were much longer.



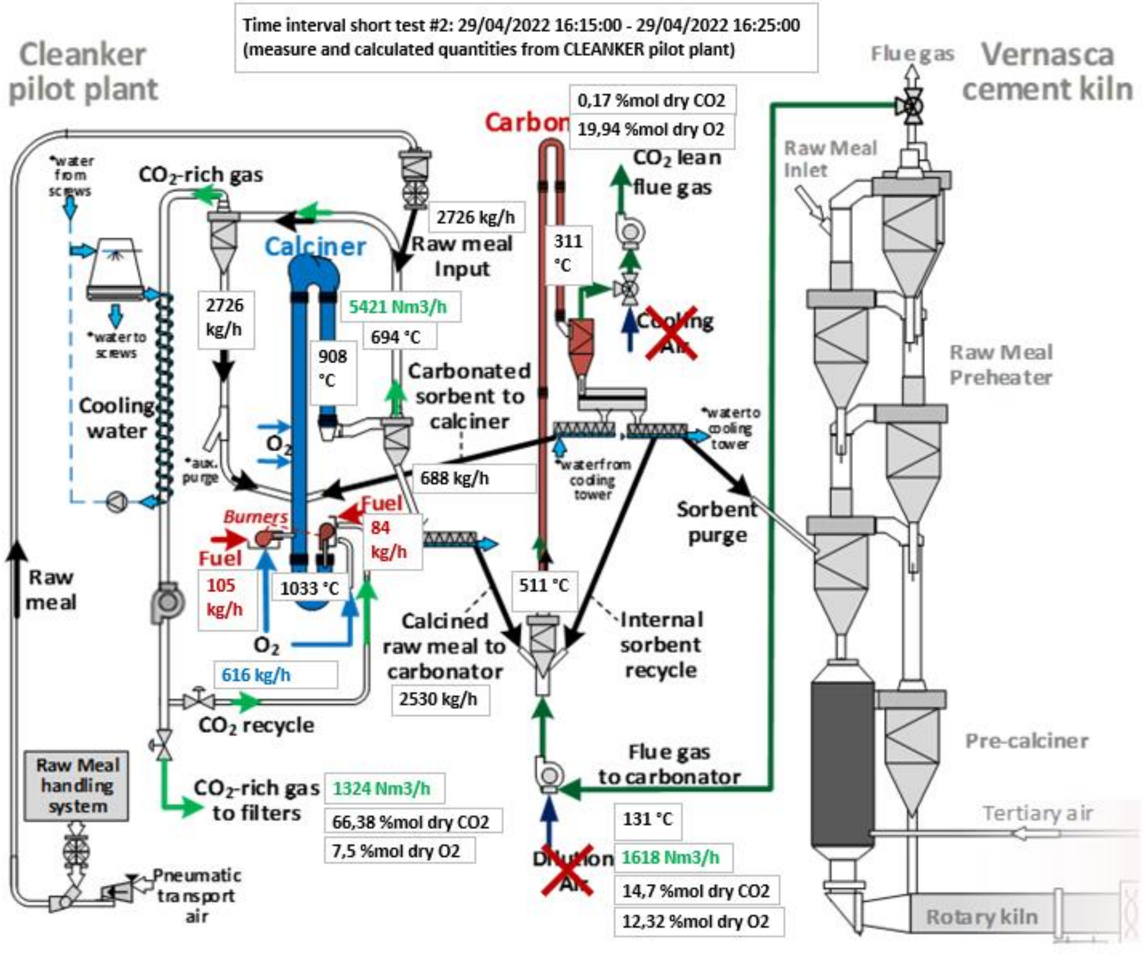
Overview: modeling tools

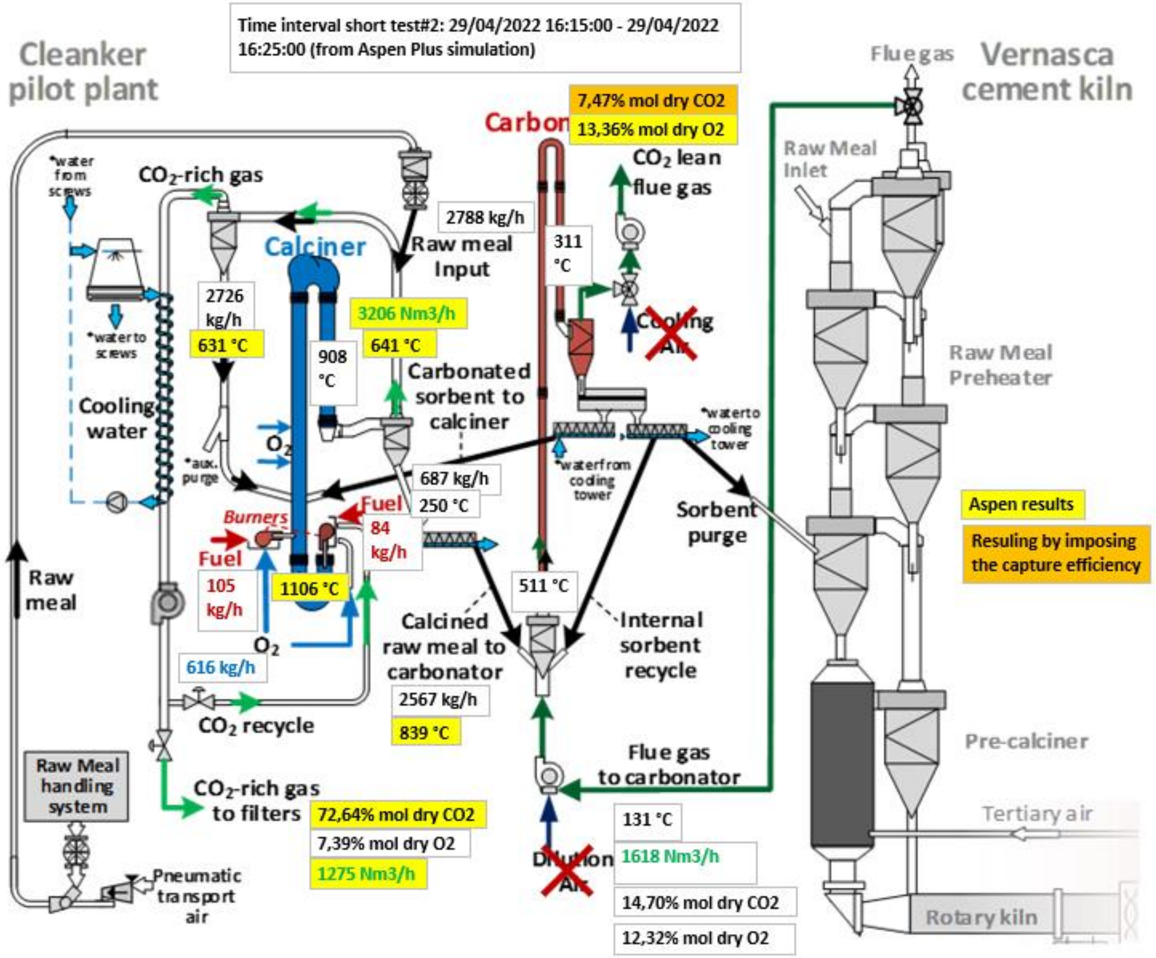
- Aspen Plus
  - Global plant simulations by POLIMI.
  - Generation of reconciled experimental data.
- 1D-model
  - In-house model code by LUT.
  - Reactor inlet conditions based on Aspen Plus simulations.
- 3D-model
  - In-house model code by LUT.
  - Fully coupled simulation of combustor, calciner, and carbonator.
  - Boundary conditions based on measurements and Aspen Plus.
- Ansys Fluent
  - Additional CFD modeling of flow fields in splash box and swirl head.



Generation of reconciled experimental data by global plant simulation

- **Several measurements inaccurate/unreliable => Aspen Plus simulations to close the balances based on analyzed solid samples and to provide consolidated measurement data.**





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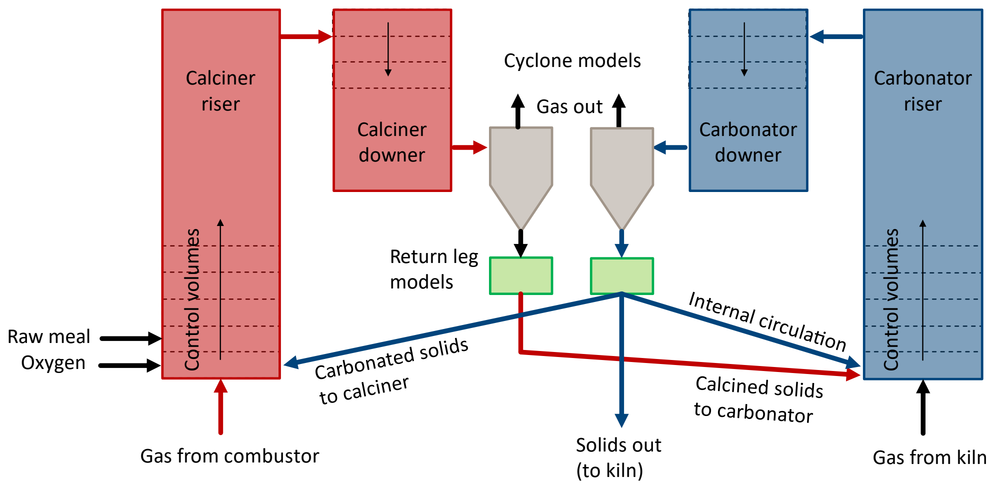
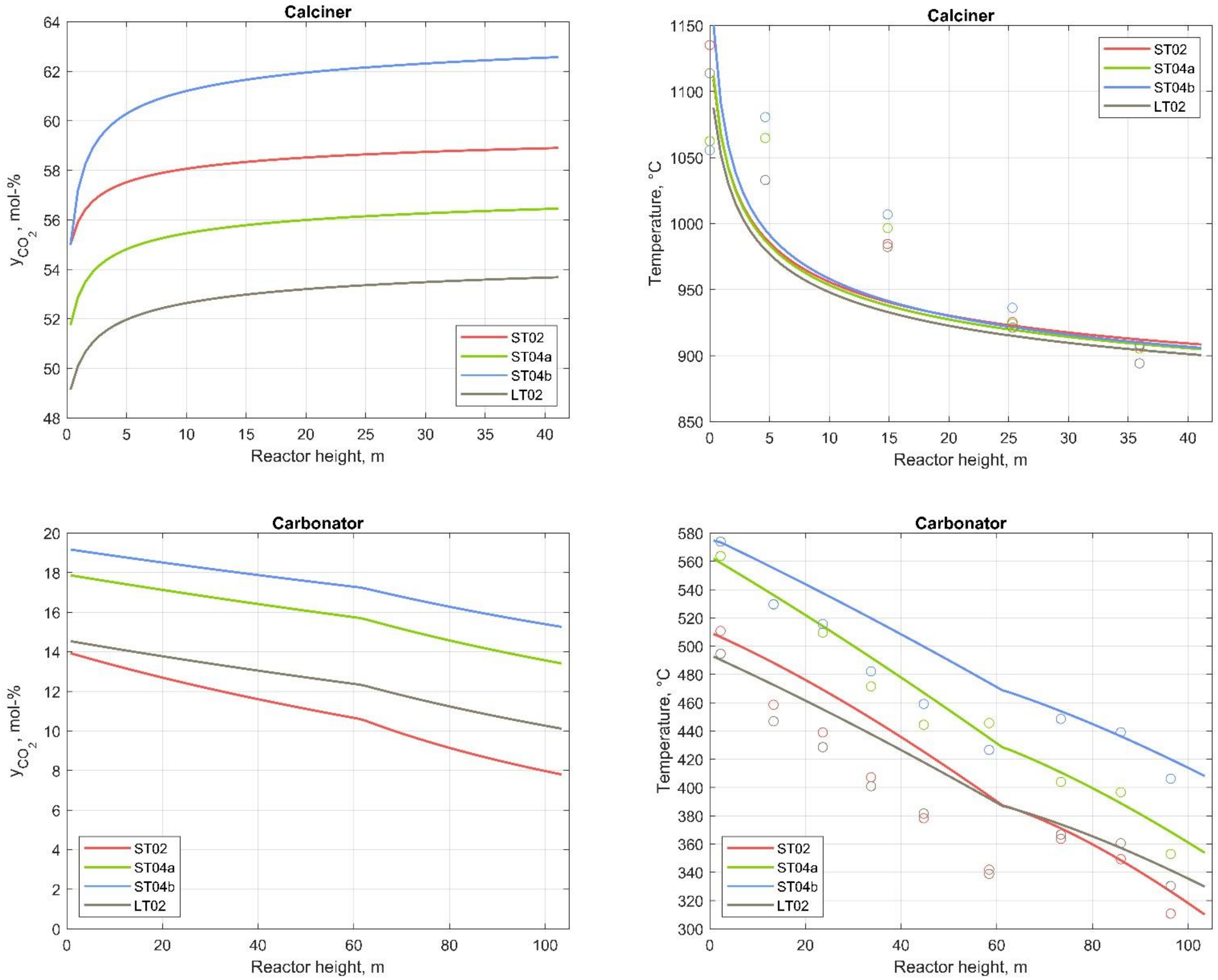
Global plant simulation: example result (ST02)

ID	Stream flow	T	qm	qn	qv	Molar composition, %vol.							Mass composition, %wt.							
		°C	kg/h	kmol/h	Nm3/h	Ar	CO2	H2O	N2	O2	SO2	O2, dry	CaO	CaCO3	CaSO4	SiO2	Al2O3	Fe2O3	MgCO3	MgO
9	Raw meal feed	60.0	2774.32	31.12	-	-	-	-	-	-	-	-	0.00	73.34	0.00	18.53	3.10	1.70	3.33	0.00
9M	Raw meal - Humidity	60.0	13.94	0.77	17.3	0.00	0.00	100.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
F-1	Fuel BU20-Vapor phase	120.0	11.16	5.11	114.6	0.00	0.00	0.46	0.36	0.00	0.00	0.00	-	-	-	-	-	-	-	-
F-1	Fuel BU20-Solid phase	120.0	93.86	7.67	-	-	-	-	-	-	-	-	0.00	0.00	0.00	1.45	0.00	0.00	0.00	0.00
OCD-BU10	Fuel BU10-Vapor phase	120.0	8.92	4.09	91.6	0.00	0.00	0.46	0.36	0.00	0.00	0.00	-	-	-	-	-	-	-	-
OCD-BU10	Fuel BU10-Solid phase	120.0	75.07	6.13	-	-	-	-	-	-	-	-	0.00	0.00	0.00	1.45	0.00	0.00	0.00	0.00
OX20-O2	Oxygen to BU20	15.0	616.00	19.25	431.5	0.00	0.00	0.00	0.00	100.00	0.00	100.00	-	-	-	-	-	-	-	-
BU10-O2	Oxygen to BU10	15.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
IJ10	Post-combustion oxygen-1	15.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
IJ11	Post-combustion oxygen-1	15.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
AT20-AIR	Atomizing air BU20	15.0	32.30	1.12	25.1	0.00	0.00	0.00	79.00	21.00	0.00	21.00	-	-	-	-	-	-	-	-
AT10-O2	Atomizing oxygen BU10	15.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
17	False air calciner-1	15.0	113.70	3.94	88.3	0.00	0.00	0.00	79.00	21.00	0.00	21.00	-	-	-	-	-	-	-	-
17-A	False air calciner-2	15.0	100.00	3.47	77.7	0.00	0.00	0.00	79.00	21.00	0.00	21.00	-	-	-	-	-	-	-	-
17-B	False air calciner-3	15.0	100.00	3.47	77.7	0.00	0.00	0.00	79.00	21.00	0.00	21.00	-	-	-	-	-	-	-	-
17-C	False air calciner-4	15.0	100.00	3.47	77.7	0.00	0.00	0.00	79.00	21.00	0.00	21.00	-	-	-	-	-	-	-	-
DU24-2	CO2 rich gas recycled to calciner	471.0	3348.38	93.80	2102.3	0.00	56.36	16.42	20.23	6.89	0.10	8.25	-	-	-	-	-	-	-	-
DU24-2	CO2 rich gas recycled to calciner-Solid phase	0.0	0.00	0.00	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	CO2 rich gas to filters-gas phase	482.5	2160.85	60.53	1356.7	0.00	56.36	16.42	20.23	6.89	0.10	8.25	-	-	-	-	-	-	-	-
7	CO2 rich gas to filters-solid phase	0.0	0.00	0.00	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
DU31	Flue gas from BU20 to BU10-gas phase	1163.4	4214.02	120.69	2704.9	0.00	50.11	16.98	19.05	13.75	0.10	16.57	-	-	-	-	-	-	-	-
DU31	Flue gas from BU20 to BU10-solid phase	1163.4	1.37	0.02	-	-	-	-	-	-	-	-	0.00	0.00	0.00	100.00	0.00	0.00	0.00	0.00
PR10-1	CO2 rich gas calciner outlet-gas phase	908.0	5247.06	145.53	3261.7	0.00	59.02	16.88	17.69	6.31	0.10	7.59	-	-	-	-	-	-	-	-
PR10-1	CO2 rich gas calciner outlet-solid phase	908.0	2565.42	41.28	-	-	-	-	-	-	-	-	52.12	12.05	0.00	26.67	4.44	2.44	0.00	2.28
DU20-3	CO2 rich gas calc. outlet after raw meal inj. (gas)	627.9	5409.23	150.87	3381.3	0.00	57.66	16.80	18.88	6.57	0.10	7.89	-	-	-	-	-	-	-	-
DU20-3	CO2 rich gas calc. outlet after raw meal inj. (solid)	627.9	2726.10	31.12	-	-	-	-	-	-	-	-	0.00	74.64	0.00	18.86	3.15	1.73	0.00	1.62
22	Solid calciner inlet-Raw meal	627.9	2726.10	31.12	-	-	-	-	-	-	-	-	0.00	74.64	0.00	18.86	3.15	1.73	0.00	1.62
13	Solid calciner inlet-from carbonator	250.0	687.00	10.12	-	-	-	-	-	-	-	-	36.95	30.25	0.00	24.42	4.07	2.23	0.00	2.09
SOL2CALC	Solid calciner inlet-total	561.2	3413.10	41.24	-	-	-	-	-	-	-	-	7.44	65.70	0.00	19.98	3.34	1.83	0.00	1.71
11	Solid from calciner to carbonator (@carb. inlet)	839.2	2565.42	41.28	-	-	-	-	-	-	-	-	52.12	12.05	0.00	26.67	4.44	2.44	0.00	2.28
19	Carbonator inlet gas-gas phase	131.0	2185.69	72.19	1617.9	0.00	14.04	4.50	69.70	11.77	0.00	12.32	-	-	-	-	-	-	-	-
19	Carbonator inlet gas-solid phase	0.0	0.00	0.00	-	-	-	-	-	-	-	-	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
12	Gas/solid mixture at carbonator inlet-gas phase	511.0	2185.69	72.19	1617.9	0.00	14.04	4.50	69.70	11.77	0.00	12.32	-	-	-	-	-	-	-	-
12	Gas/solid mixture at carbonator inlet-solid phase	511.0	2565.45	41.28	-	-	-	-	-	-	-	-	52.12	12.05	0.00	26.67	4.44	2.44	0.00	2.28
16	False air carbonator	15.0	0.00	0.00	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.00	-	-	-	-	-	-	-	-
S-7	Gas/solid mixture at carbonator outlet-gas phase	311.0	1948.89	66.81	1497.3	0.00	7.12	4.86	75.31	12.71	0.00	13.36	-	-	-	-	-	-	-	-
S-7	Gas/solid mixture at carbonator outlet-solid phase	311.0	2802.25	41.28	-	-	-	-	-	-	-	-	36.95	30.25	0.00	24.42	4.07	2.23	0.00	2.09

1D model results

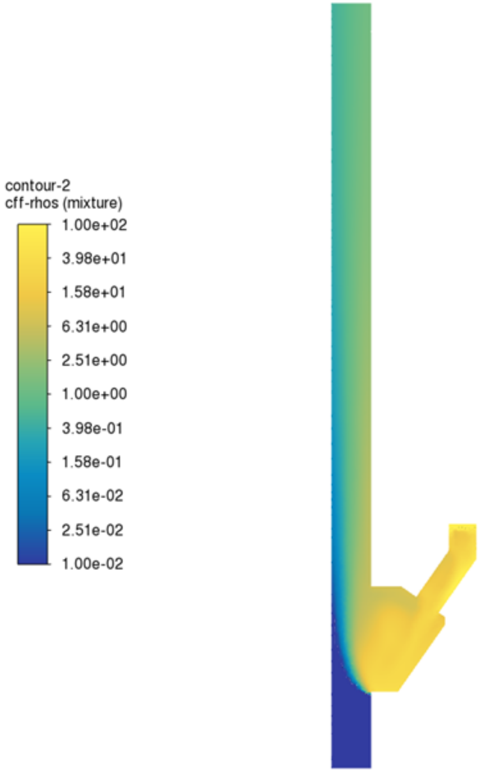


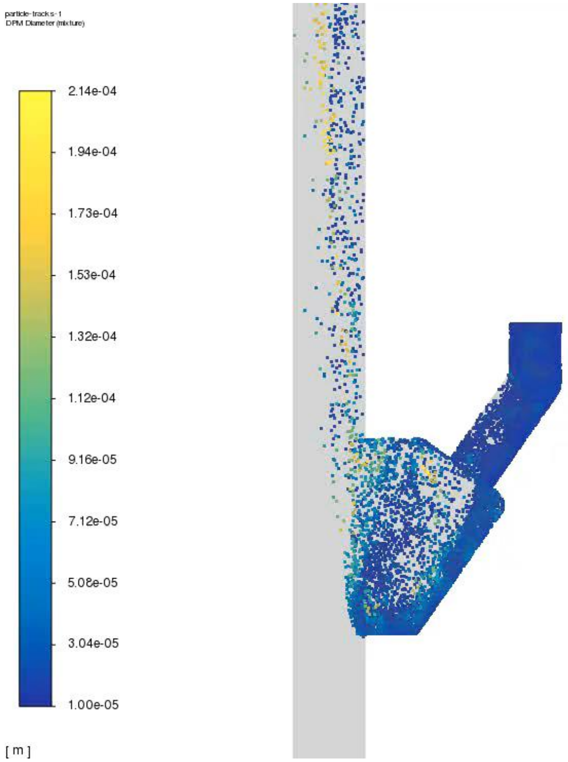


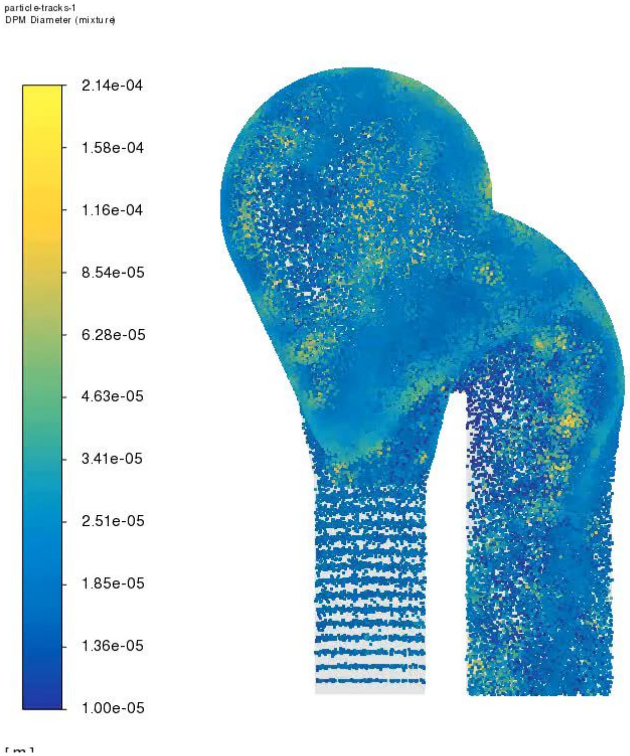
- **The riser and downer sections of both reactors are discretized to control volumes along the length of the reactor.**
- **Inlet conditions based on reconciled experimental data.**

CFD modeling of splash box and swirl head

- Mostly plug flow conditions in entrained flow mode, except the solid inlet point and the turning point.
- The higher concentration of solids increases the local reaction rates, especially near to the splash box.

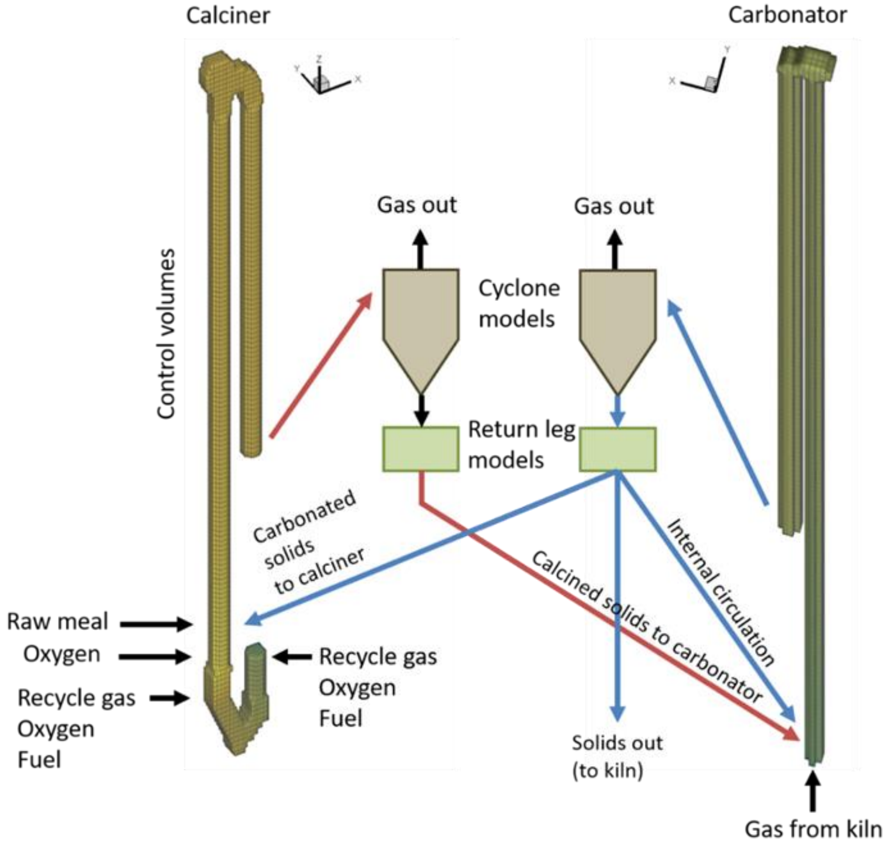




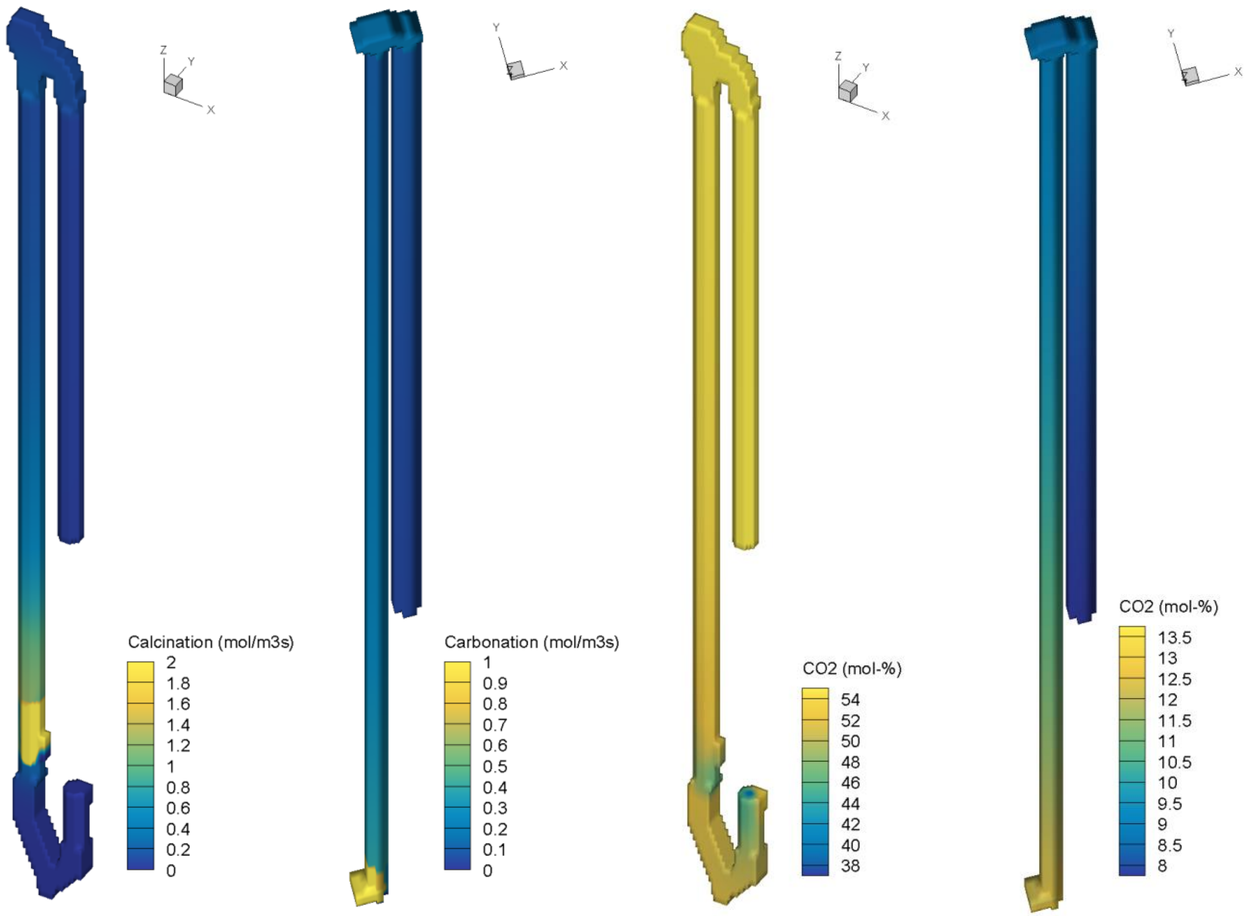


3D modeling

Model frame

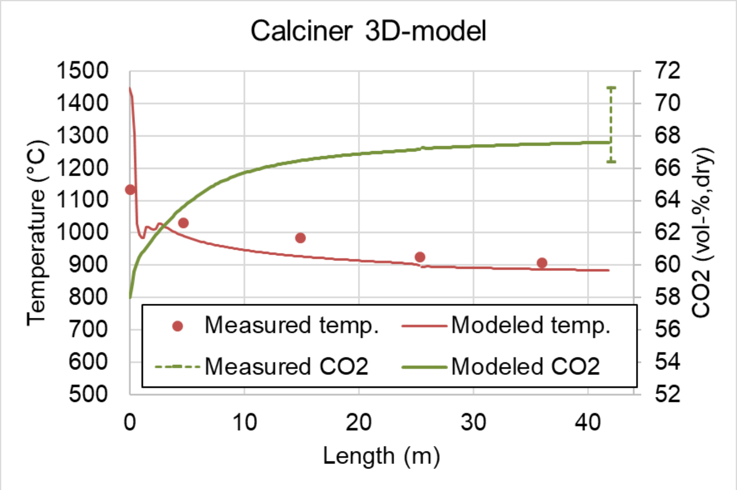


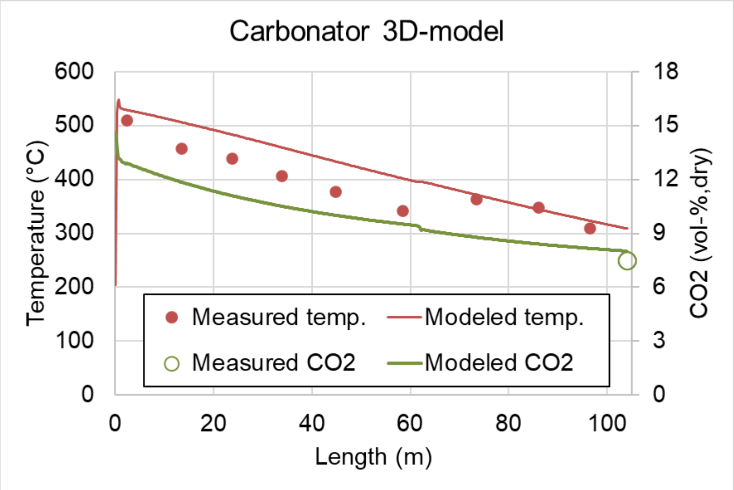
Example 3D-model results (ST02)

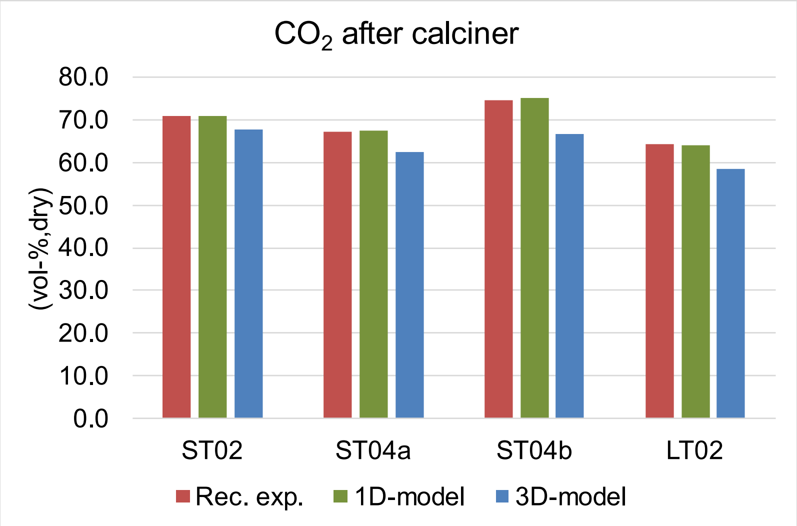


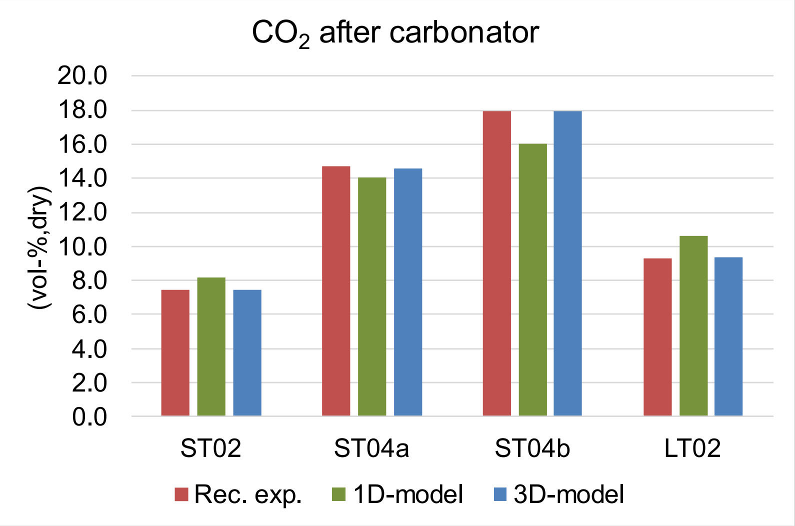
Tuning and validation

Test case ST02	Raw meas.	Rec. exp.	1D-model	3D-model
Gas flow after calciner (kg/s)	1.85	1.46	1.45	1.52
Temperature (°C)	908	908	908	884
O_2 (vol-%)	7.5	7.6	7.6	7.2
CO_2 (vol-%)	66.4	71.0	70.9	67.8
Calcination degree (%)		88.5	87.0	87.5
Gas flow after carbonator (kg/s)		0.54	0.55	0.54
Temperature (°C)	311	311	310	309
O_2 (vol-%)		13.4	13.3	13.4
CO_2 (vol-%)		7.5	8.2	7.5
CO_2 capture efficiency (%)		53.1	48.1	53.0









Rec. exp. = reconciled experimental data by global plant simulation

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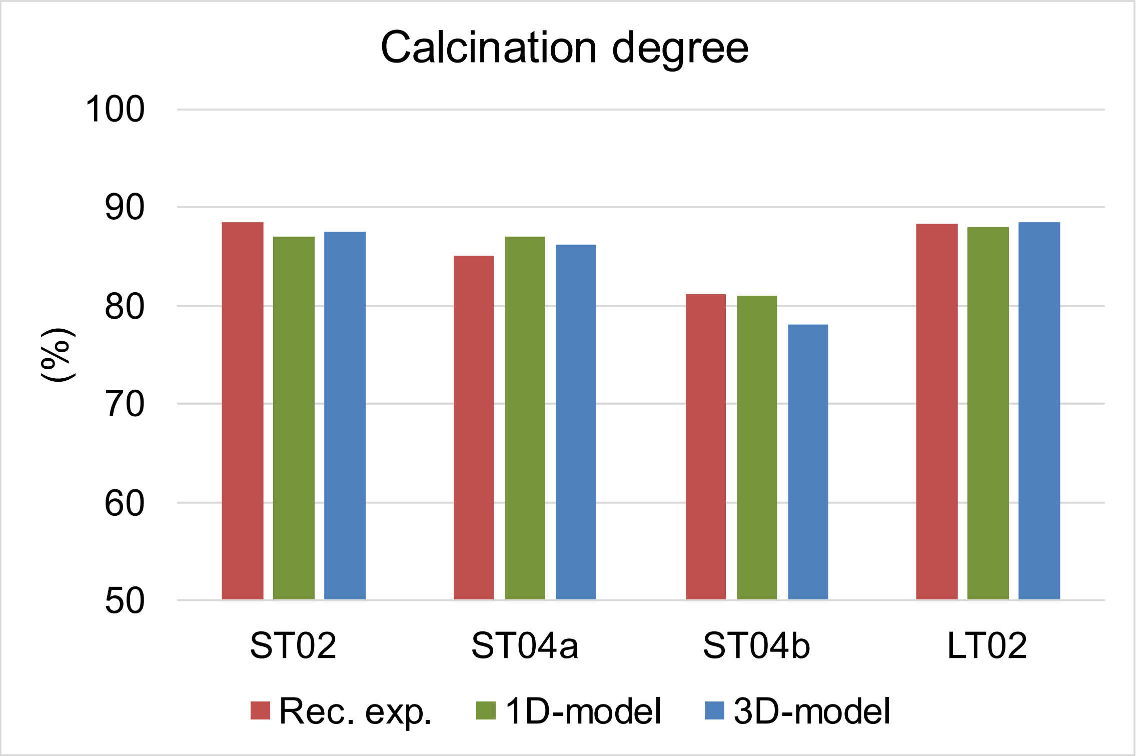
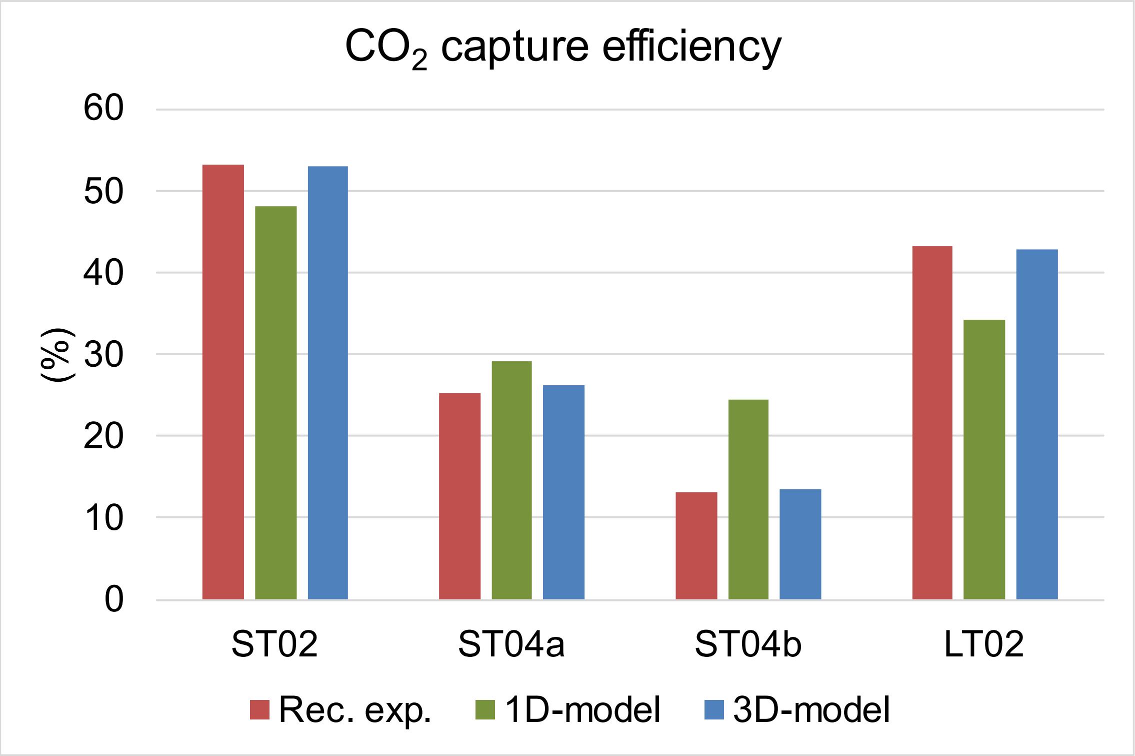
Calcination degree and carbon capture efficiency





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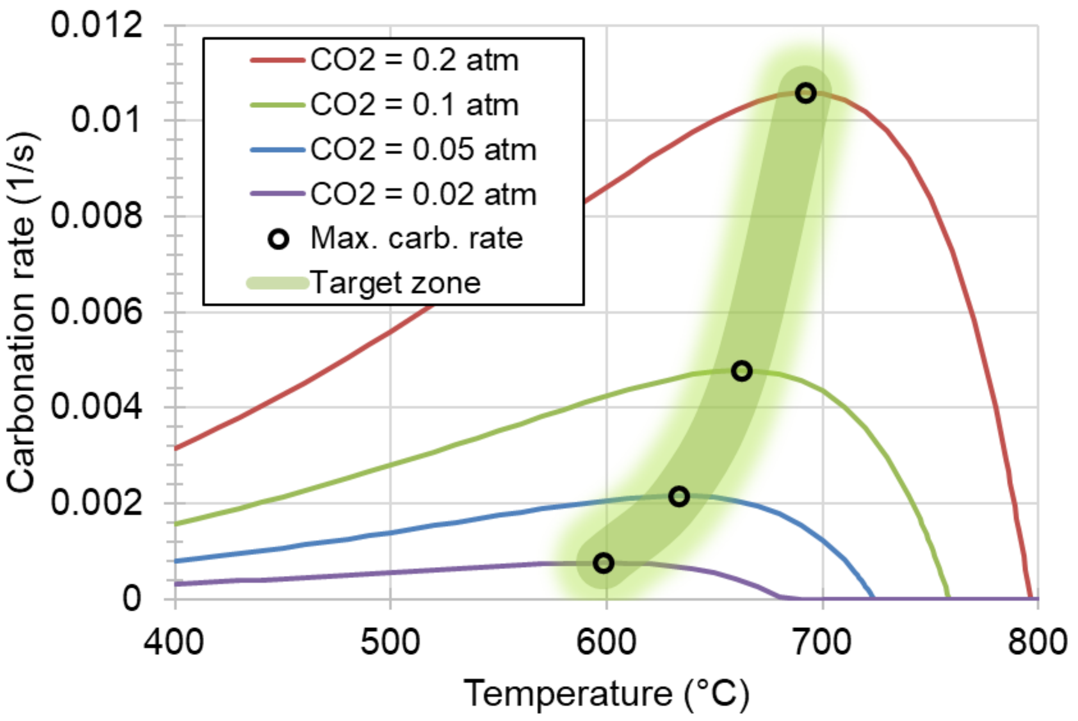
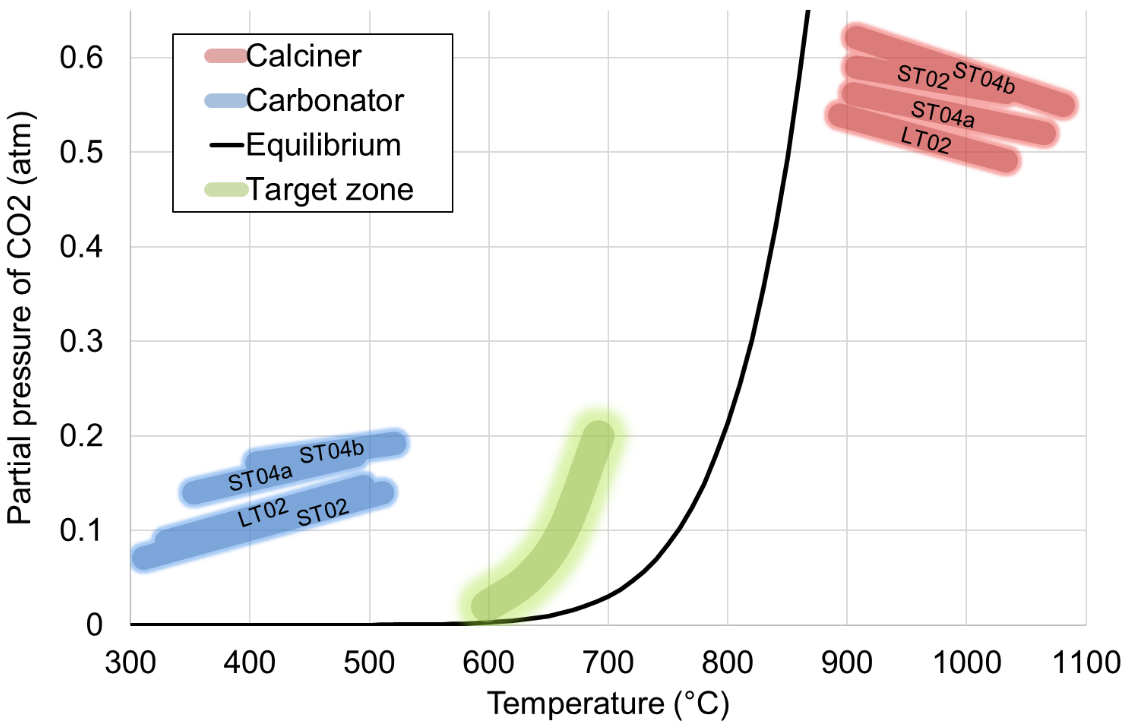
Analysis of carbon capture efficiency



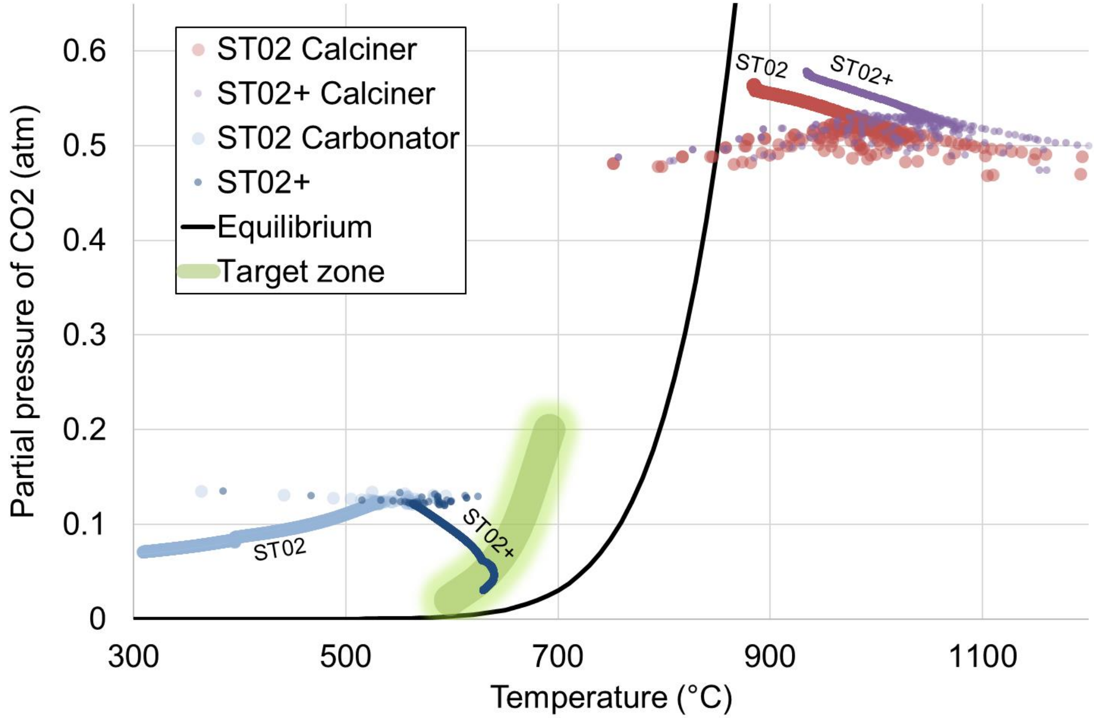


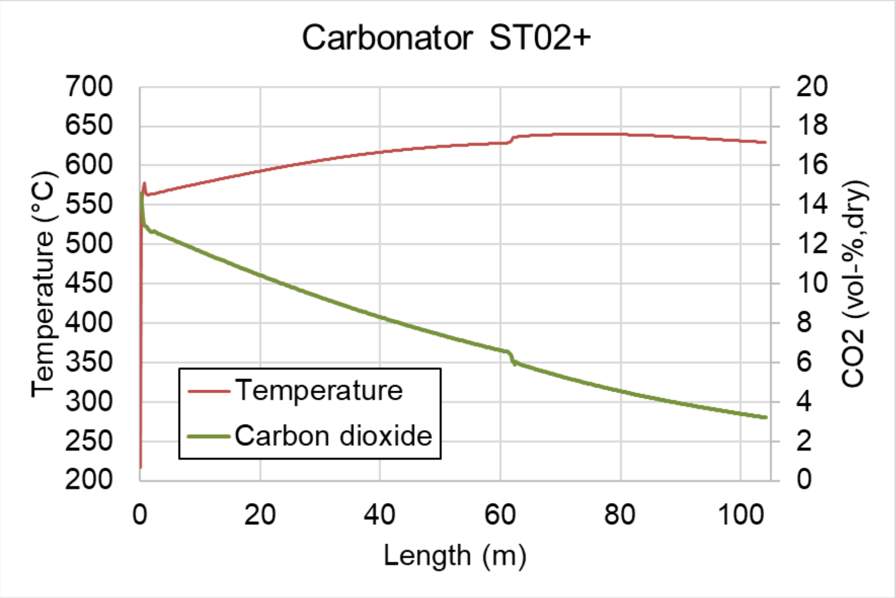
$$\frac{dX_{carb}}{dt} = c_{carb}\, A_{carb}\, exp\left(\frac{-E_{a,carb}}{RT}\right) \left(p_{CO2} - p_{eq}\right) \left(X_{max} - X_{carb}\right)^{(2/3)}$$

Optimized carbon capture => ST02+

- Decreased gas flow to carbonator: 0.61 => 0.50 kg/s (-18%)
  - Still entrained flow mode (>18 m/s).
  - Gas/solid-ratio 1.6 => 1.9 kg/Nm3.
- Insulated carbonator: heat loss 506 => 170 kW (-66%).
- Higher fuel input to calciner: 2119 => 2340 kW (+10%).
  - Outlet O_2 7.2 => 5.6 vol-%,dry.

	ST02	ST02+
Gas flow after calciner (kg/s)	1.52	1.55
Temperature (°C)	884	934
CO_2 (vol-%,dry)	67.8	69.5
Calcination degree (%)	87.5	88.6
Gas flow after carbonator (kg/s)	0.54	0.42
Temperature (°C)	309	630
CO_2 (vol-%,dry)	7.5	3.2
CO_2 capture efficiency (%)	53.0	80.8





Conclusions

- Reconciled experimental data by global plant simulations.
- 1D- and 3D-models were tuned based on the generated data.
- With the existing tests, the carbon capture efficiency has been up to 53%.
- In the 3D-model, the carbon capture efficiency could be increased up to 80%.
    - Insulated carbonator, increased solid/gas-ratio by decreased gas flow to carbonator, increased fuel input.
- Many operational problems are related to small scale => higher capture efficiency in large scale.
- The validated models can be applied to simulate a large scale CLEANKER process.

Acknowledgments

CLEAN clinKER by calcium looping for low-CO_2 cement

CLEANKER

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