SFERA-III

Solar Facilities for the European Research Area

“Optimization and automation of the operational strategy of a CSP reactor for thermochemical hydrogen generation”

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NETWORKING

Summer School: “Smart CSP: How Smart Tools, Devices, and Software can help improve the Design and Operation of Concentrating Solar Power Technologies” - WP1 Capacity building and training activities - Cologne, Germany, September 14th-15th 2023

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Outline

1) Background
    - Thermochemical hydrogen generation
    - Astor reactor and automation
2) Simulation model
    - Basic system behavior
    - Operational parameters
3) Results on optimal operational strategy
4) Conclusions

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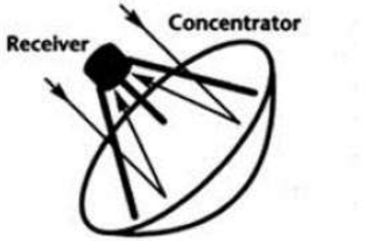
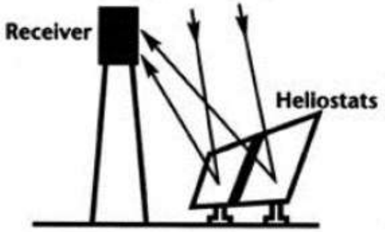
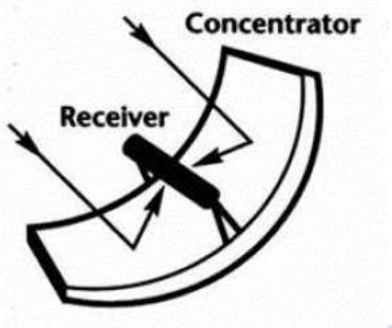
Solar thermal power plants



parabolic dish
3500 °C



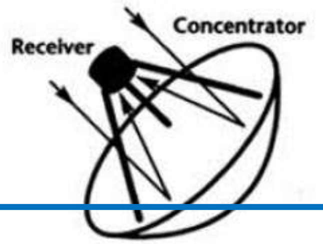
solar tower
1500 °C



parabolic trough
400 - 500 °C

Source: DLR

Solar thermal power plants



parabolic dish
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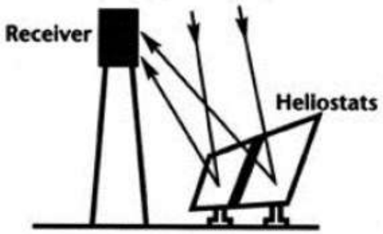
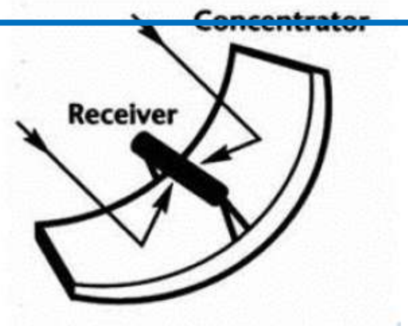


→ **thermochemical hydrogen generation**

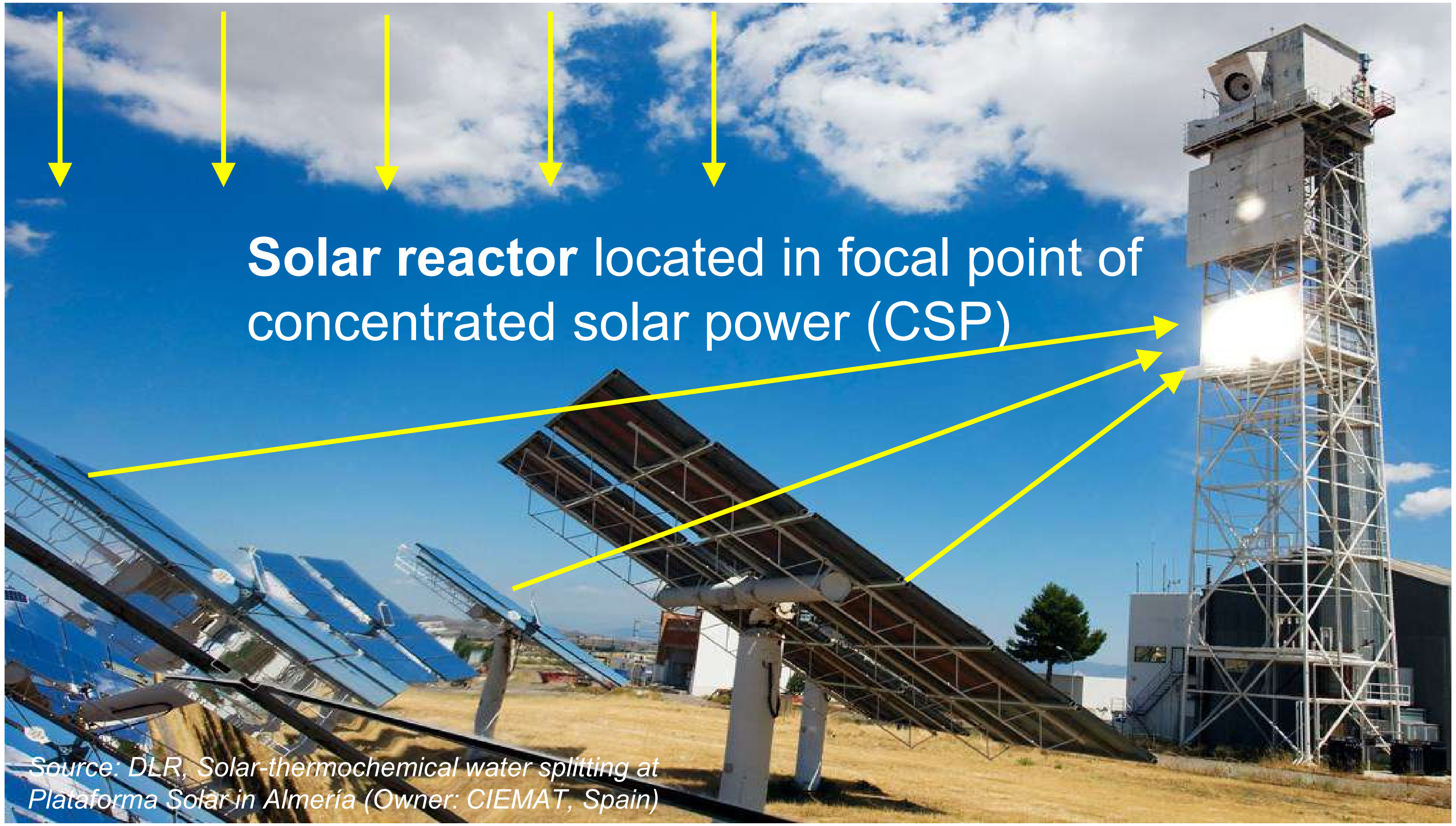
solar tower
1500 °C



parabolic trough
400 - 500 °C

Source: DLR

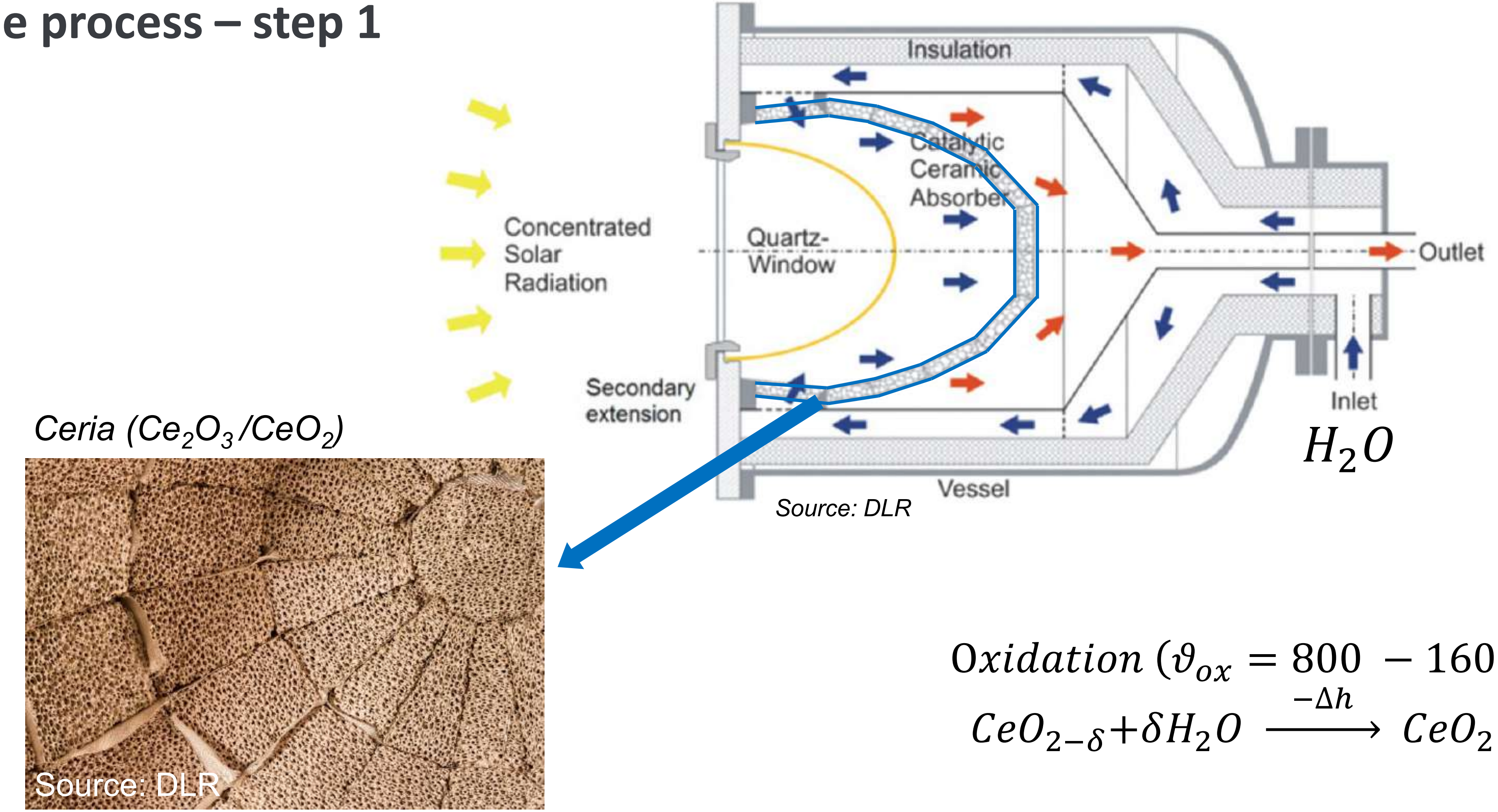
Direct thermochemical water splitting



Solar reactor located in focal point of concentrated solar power (CSP)

Source: DLR, Solar-thermochemical water splitting at Plataforma Solar in Almería (Owner: CIEMAT, Spain)

Cycle process – step 1



H_2O

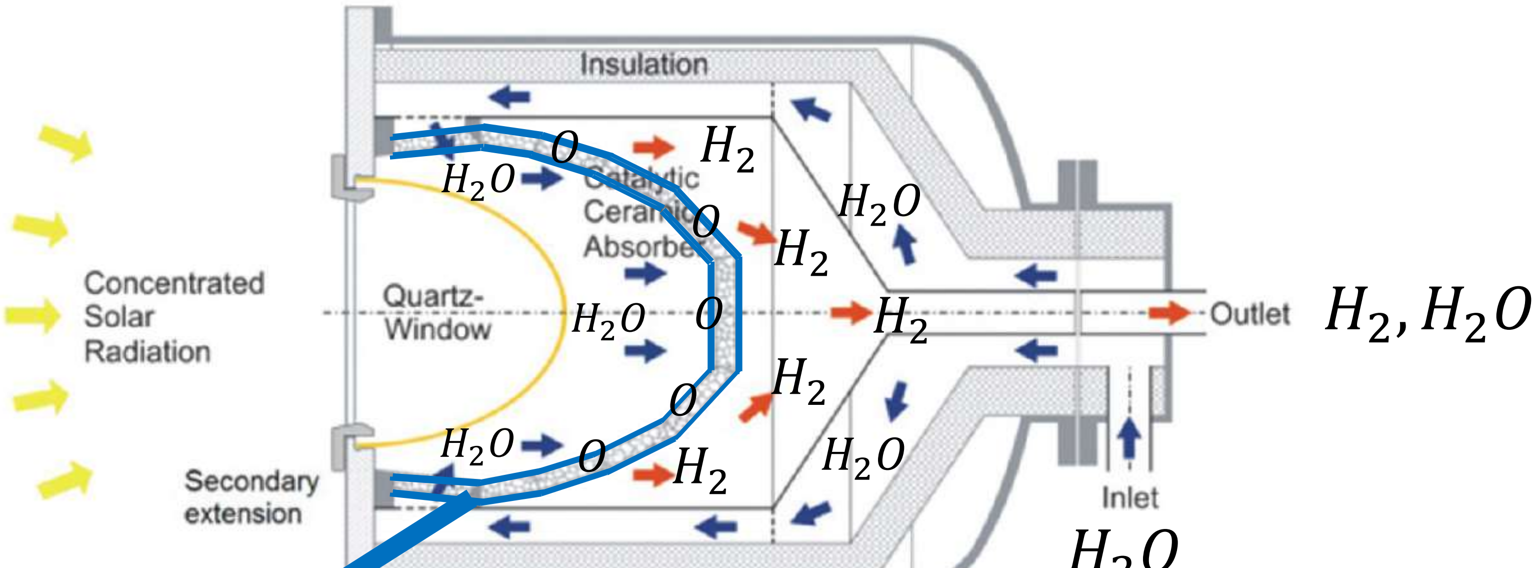
Source: DLR

Ceria (Ce_2O_3/CeO_2)

$$\mathrm{Oxidation}\ (\vartheta_{ox} = 800 - 1600\,°C):$$

$$CeO_{2-\delta} + \delta H_2O \xrightarrow{-\Delta h} CeO_2 + \delta H_2$$

Cycle process – step 1



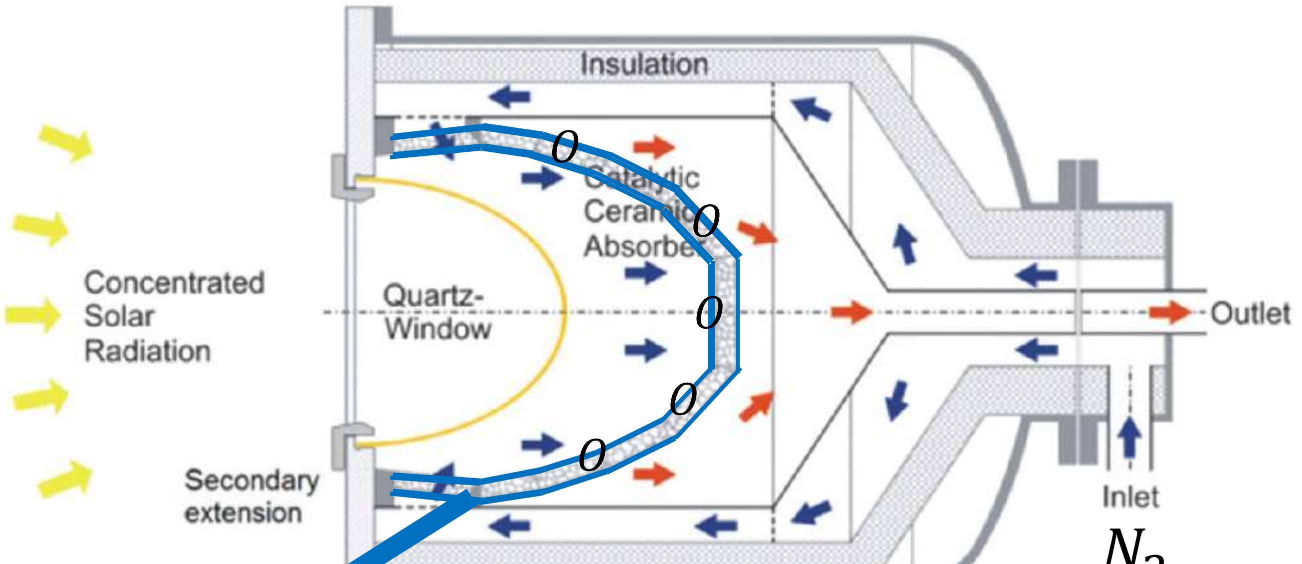
Source: DLR

Ceria (Ce_2O_3/CeO_2)

$$Oxidation\ (\vartheta_{ox} = 800\ - 1600\ °C):$$

$$CeO_{2-\delta} + \delta H_2O \xrightarrow{-\Delta h} CeO_2 \boxed{+\ \delta H_2}$$

Cycle process – step 2



Source: DLR

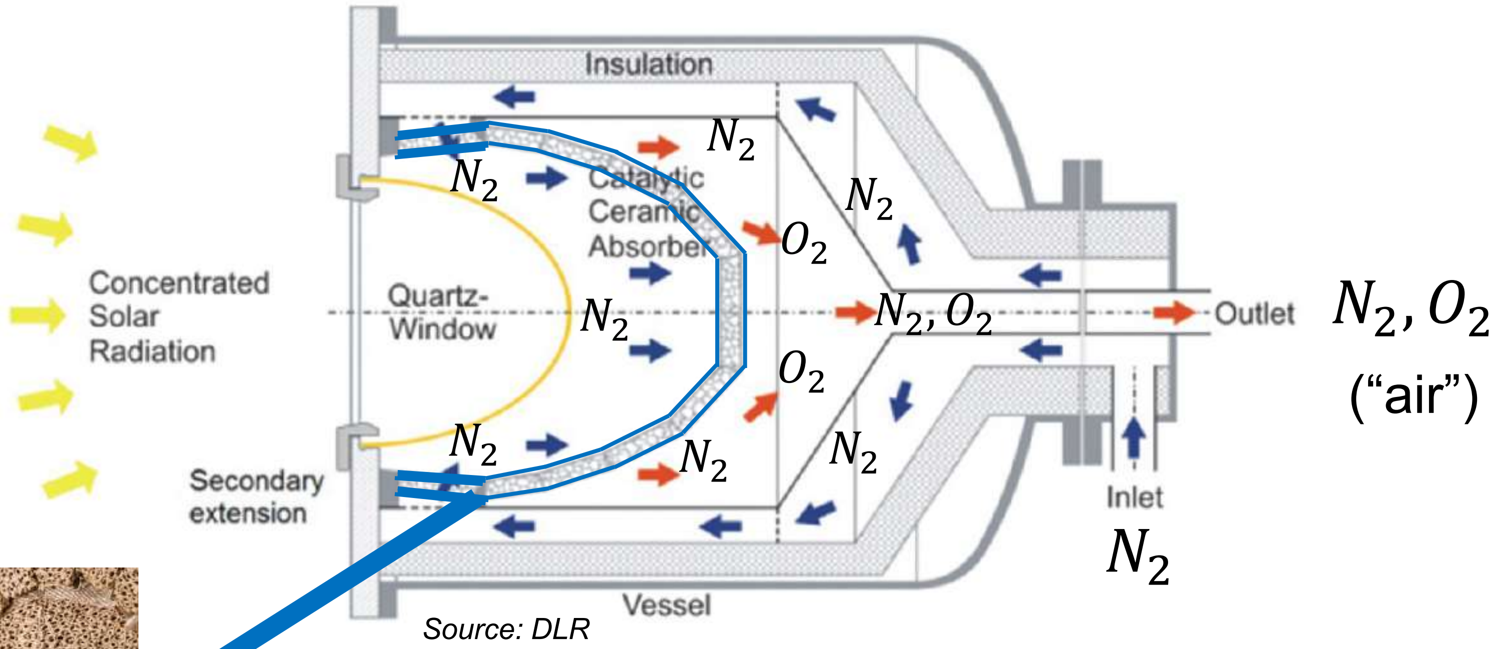
Ceria (Ce_2O_3/CeO_2)

Source: DLR

$$Reduction\ (\vartheta_{red} = 1600\ °C):$$

$$CeO_2 \xrightarrow{+\Delta h} CeO_{2-\delta} + \frac{\delta}{2} O_2$$

Cycle process – step 2



Source: DLR

N_2, O_2
("air")

Inlet N_2

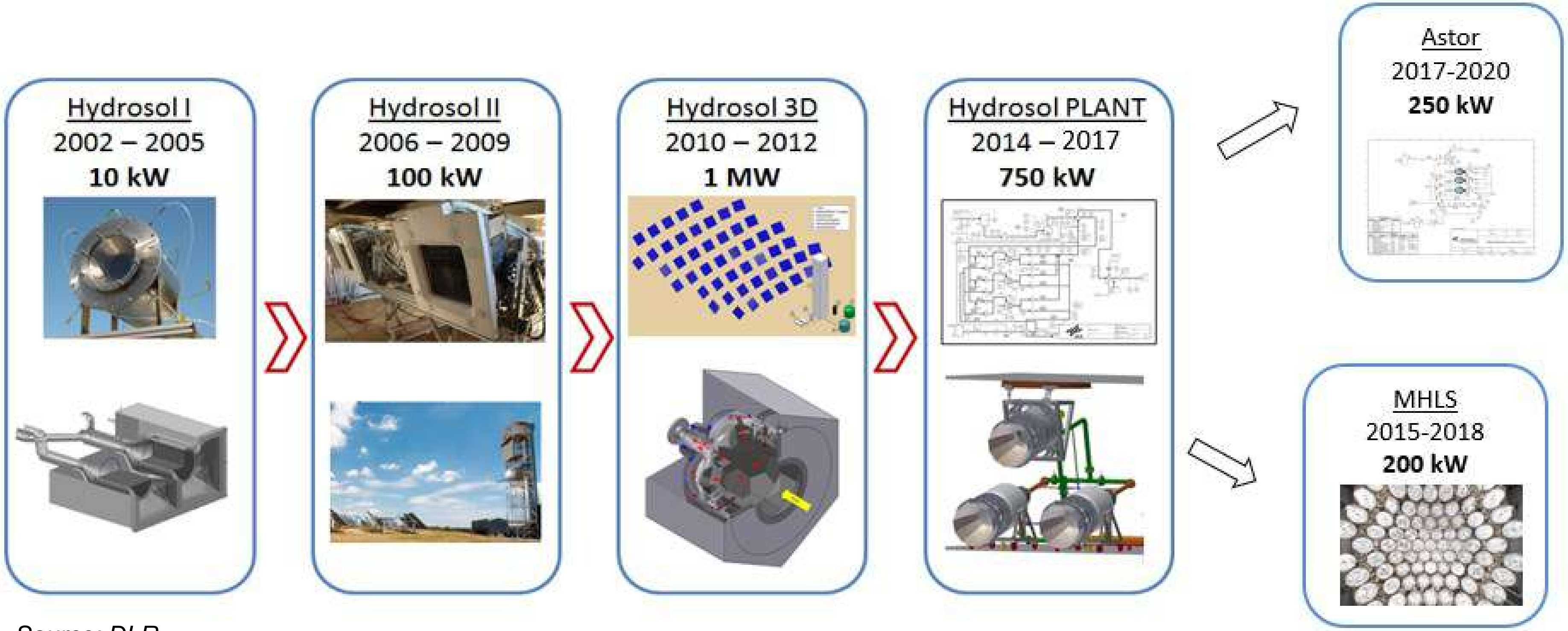
Ceria (Ce_2O_3/CeO_2)

Source: DLR

$$Reduction\ (\vartheta_{red} = 1600\ °C):$$

$$CeO_2 \xrightarrow{+\Delta h} CeO_{2-\delta} \boxed{+\frac{\delta}{2}O_2}$$

History of Hydrosol technology



Hydrosol I
2002 – 2005
10 kW

Hydrosol II
2006 – 2009
100 kW

Hydrosol 3D
2010 – 2012
1 MW

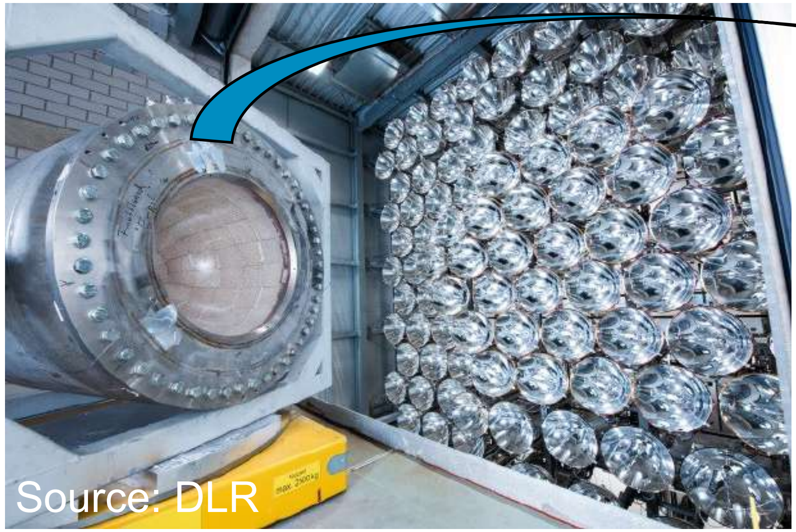
Hydrosol PLANT
2014 – 2017
750 kW

Astor
2017-2020
250 kW

MHLS
2015-2018
200 kW

Source: DLR

ASTOR reactor



Source: DLR

Astor reactor, Synlight lab…

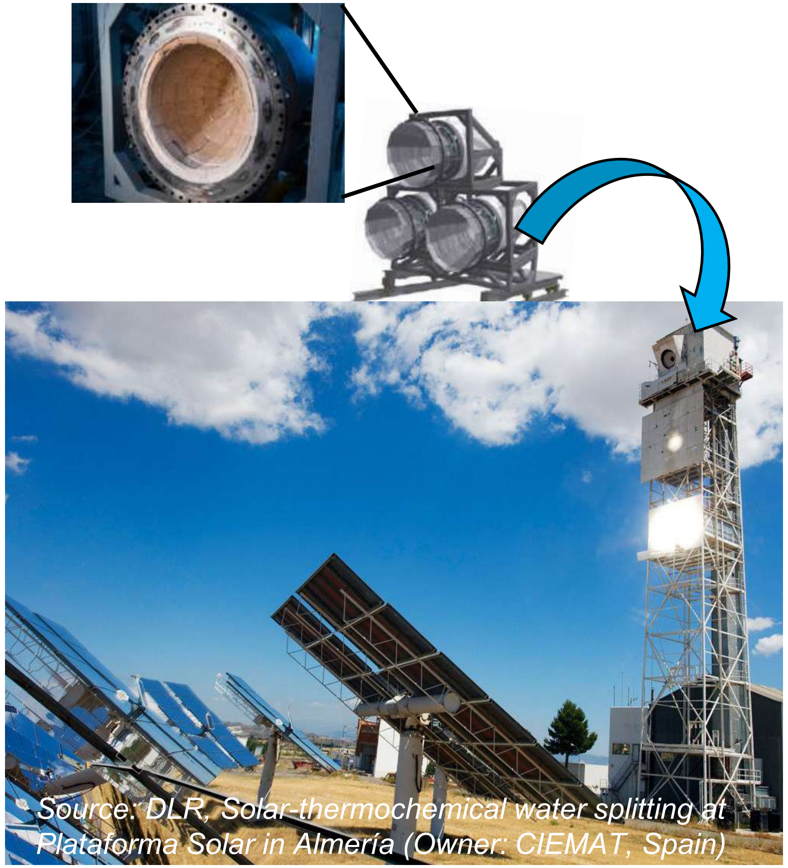
Source: DLR

…and solar tower in Julich, Germany

250 kW prototype reactor

- Automation and control
- Optimization of material, design + operational strategy
- Modeling of reactor and process

Automation



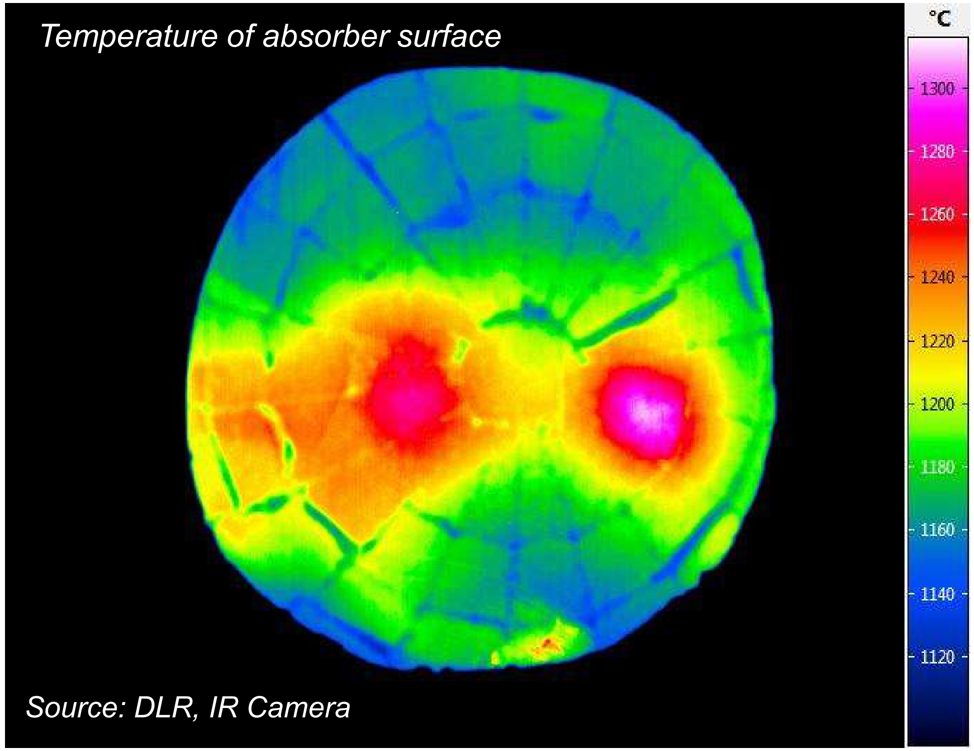
Source: DLR, Solar-thermochemical water splitting at Plataforma Solar in Almería (Owner: CIEMAT, Spain)

Heliostat field control
- Power input
  → operating temperature

Control for three reactors
- One physical + two virtual reactors
- Realtime model
  → Hardware-in-the-Loop

DNI prognosis
  - Temporarily shadowing
  - Adaption of optimal operation

Automation and control



Temperature feedback control

- Process behavior depends on operating point (temp, mass flows)
- Surface temperature as control variable
- Backside temperature as measured variable

→ Advanced gain scheduling or model predictive control

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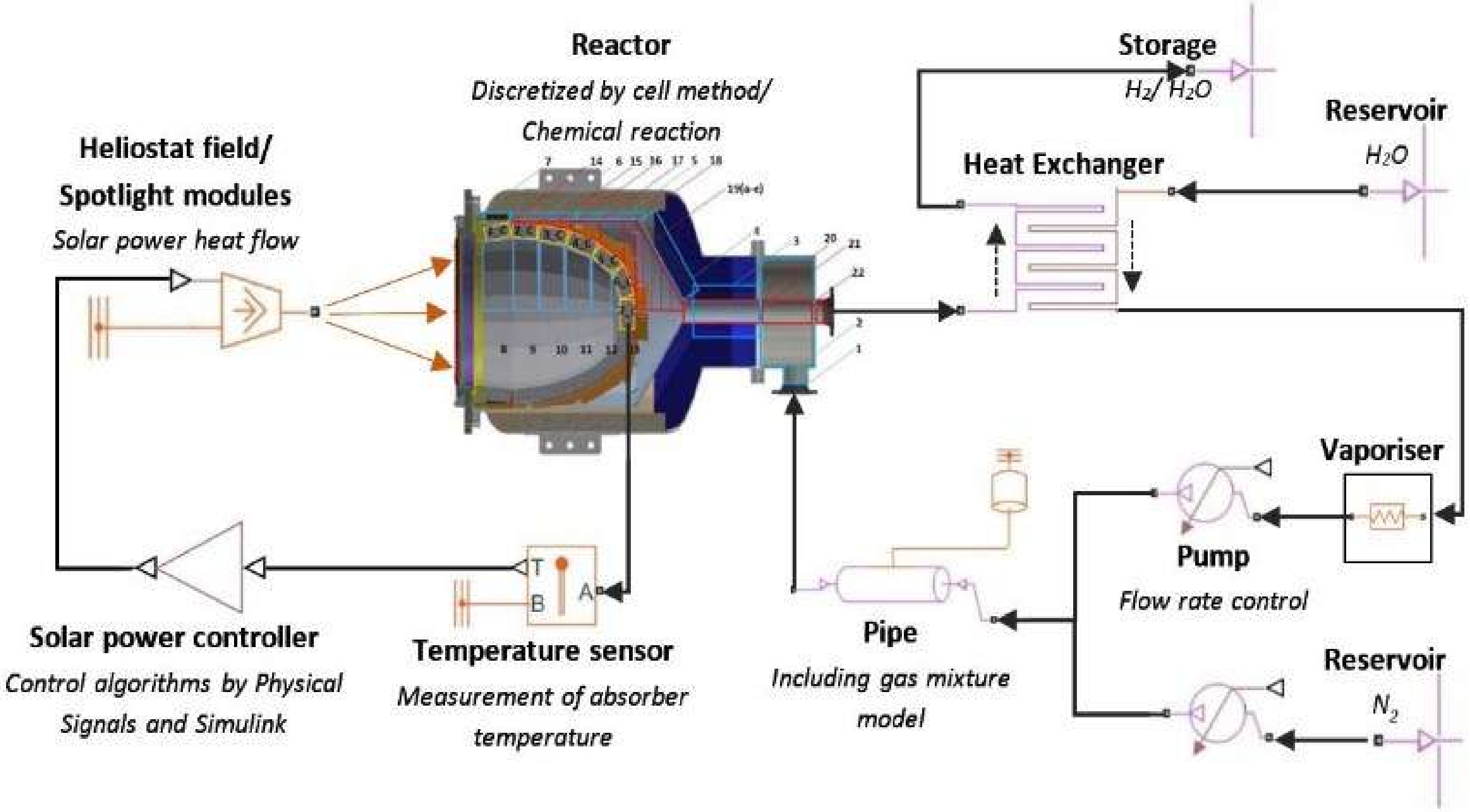
Simulation model


Reactor
Discretized by cell method/
Chemical reaction

Storage
H_2/ H_2O

Reservoir
H_2O

Heat Exchanger

Heliostat field/
Spotlight modules
Solar power heat flow

Vaporiser

Pump
Flow rate control

Reservoir
N_2

Solar power controller
Control algorithms by Physical
Signals and Simulink

Temperature sensor
Measurement of absorber
temperature

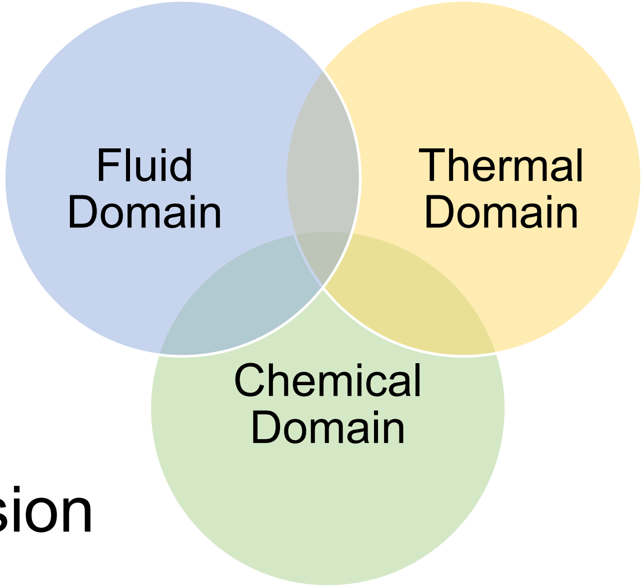
Pipe
Including gas mixture
model

→ Physical modelling, spatial discretization

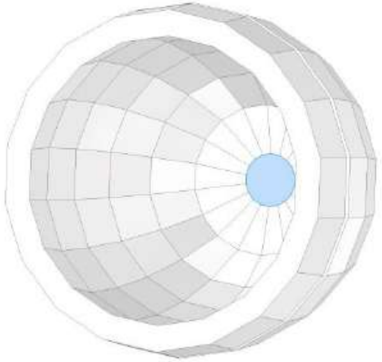
→ Discretized system of PDEs with additional constraints leads to DAE of order ~3500

Multiphysical model

- Some processes are nonlinear (chem. reaction, flow through porous media)
- Some processes have fast dynamic (valves, chemical reaction), others are slow (temperature change)
- Radiosity distribution, reflection, absorption, transmission



Receiver consists of 109 blocks

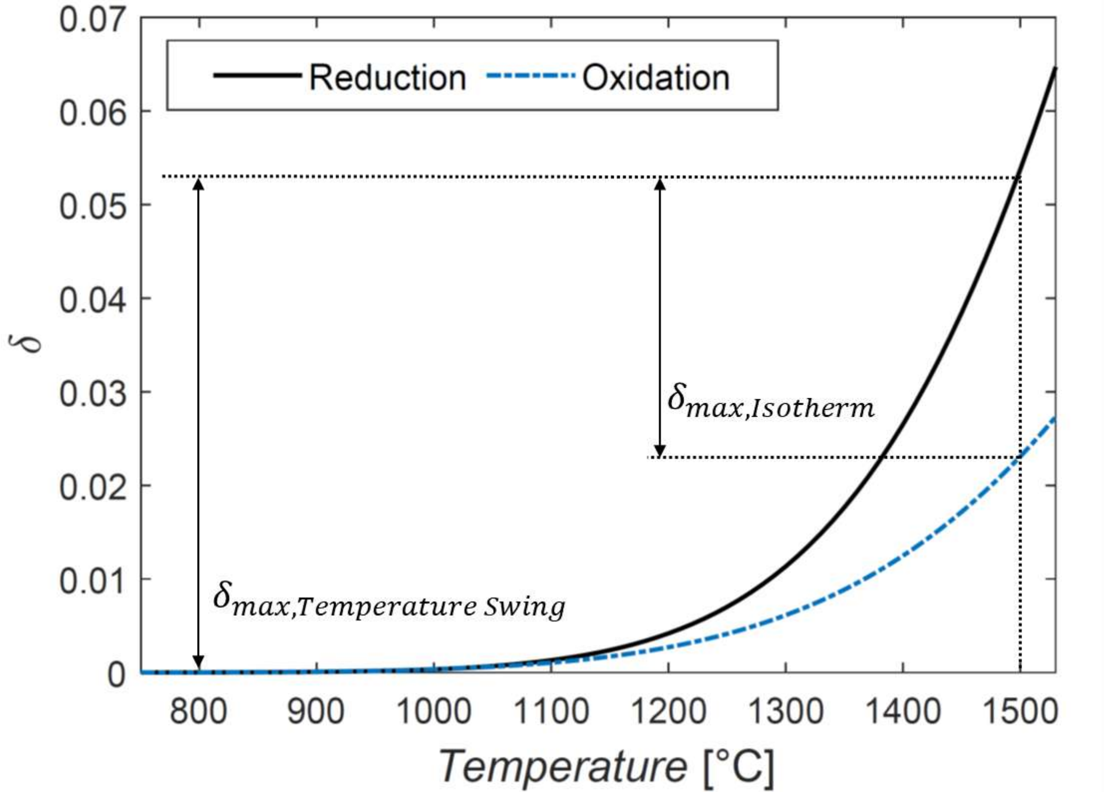


Temperature dependent properties

Source: DLR

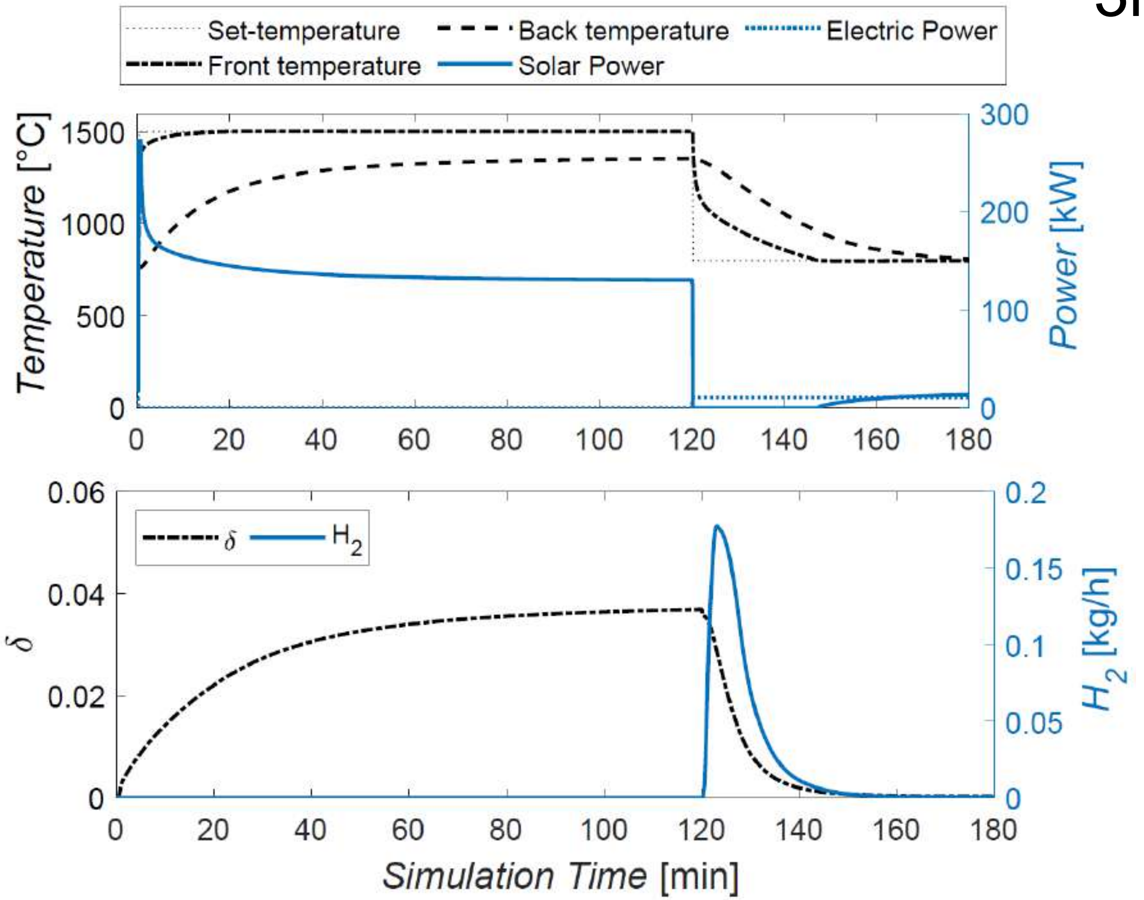
Thermochemical relations of Ceria redox cycling

Non-stoichiometric coefficient $\delta(T)$



- Reduction extent δ from $CeO_{2-\delta}$
- Equilibrium values for $p_{O_2} = 10^{-5}$ bar at reduction
- Value of δ_{max} indicates hydrogen generation potential
- Isothermal operation only reasonable at high temperatures + steam flows
- Large temp-swings relate to high δ_{max}
- Larger swings require longer cycles

Basic system behavior



3h temperature swing cycle with $\Delta\vartheta = 700\,°C$

- 2h reduction at $\vartheta_{red} = 1500\,°C$ with N_2 flow of 100 kg/h
- 1h oxidation at $\vartheta_{ox} = 800\,°C$ with steam flow of 15 kg/h
- 27 g H_2 are generated in the cycle
- Back temperature needs long until steady state
- Most H_2 is generated within first 10 minutes of oxidation

Operational parameters for optimization

Process parameter	Lower bound	Upper bound
ϑ_{red}	1200 °C	1400 / 1500 / 1600 °C
ϑ_{ox}	800 °C	1400 / 1500 / 1600 °C
t_{red}	30 s	900 s
t_{ox}	30 s	900 s
$\dot{m}_{N_2}$	100 kg/h	300 kg/h
$\dot{m}_{H_2O}$	15 kg/h	300 kg/h

Plant efficiency is used as cost function

$$\eta_{plant} = \frac{m_{H_2} \cdot HHV_{H_2}}{Q_{solar} + E_{el,vap} + m_{N_2} \cdot e_{N_2}}$$

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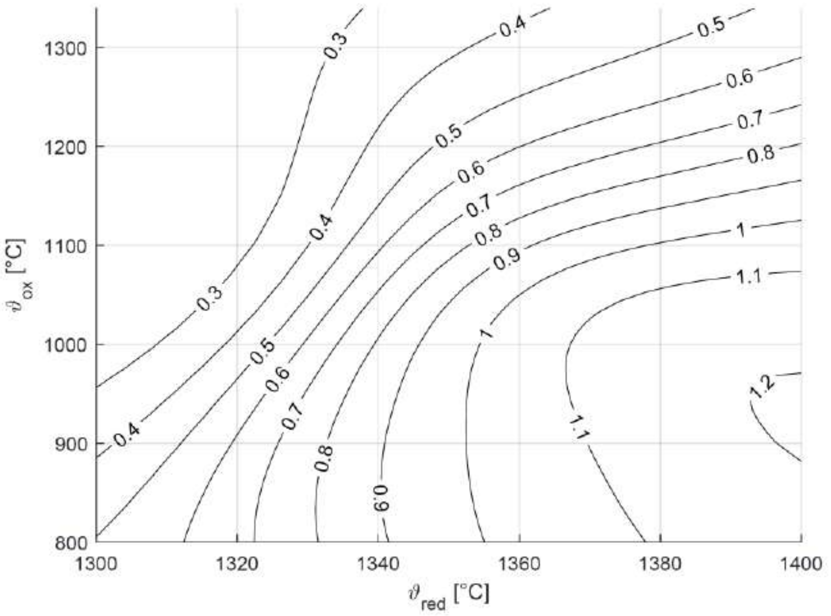
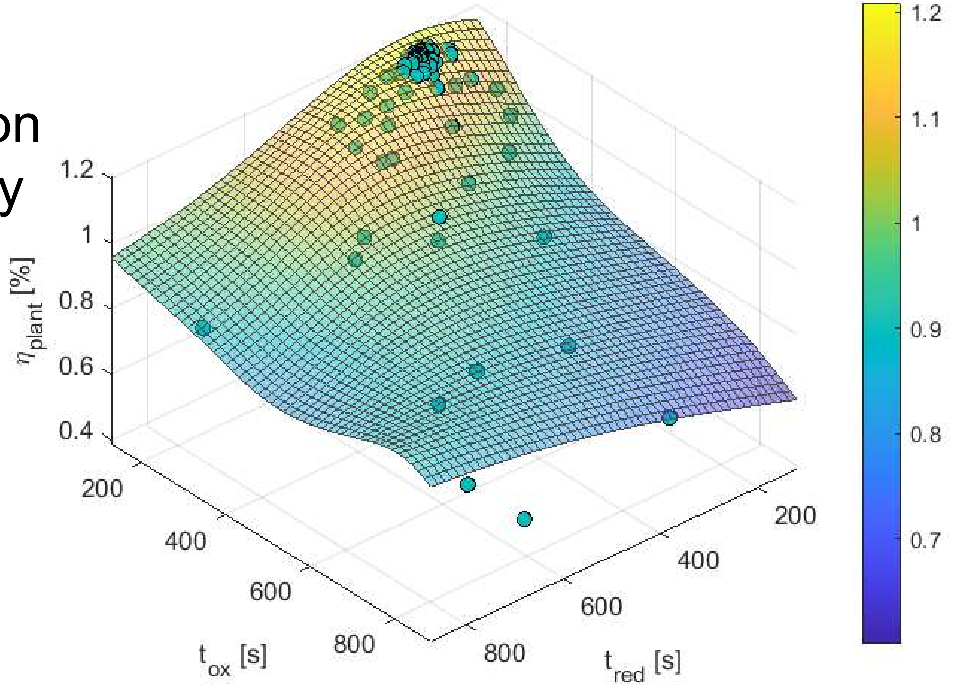
Optimal parameters for $\vartheta_{max} = 1400\ °C$



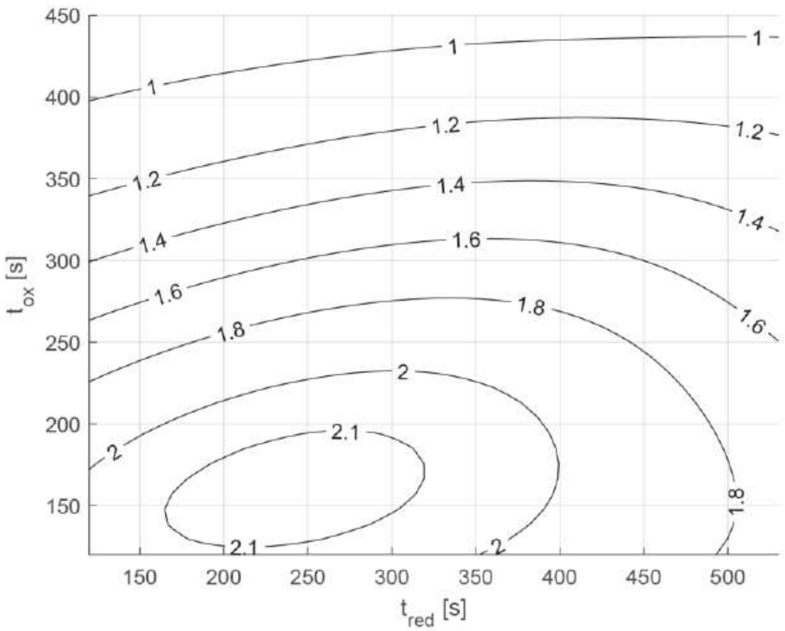
Contour plot of plant efficiency
(for temperatures)

3D model function
of plant efficiency
(for cycle times)



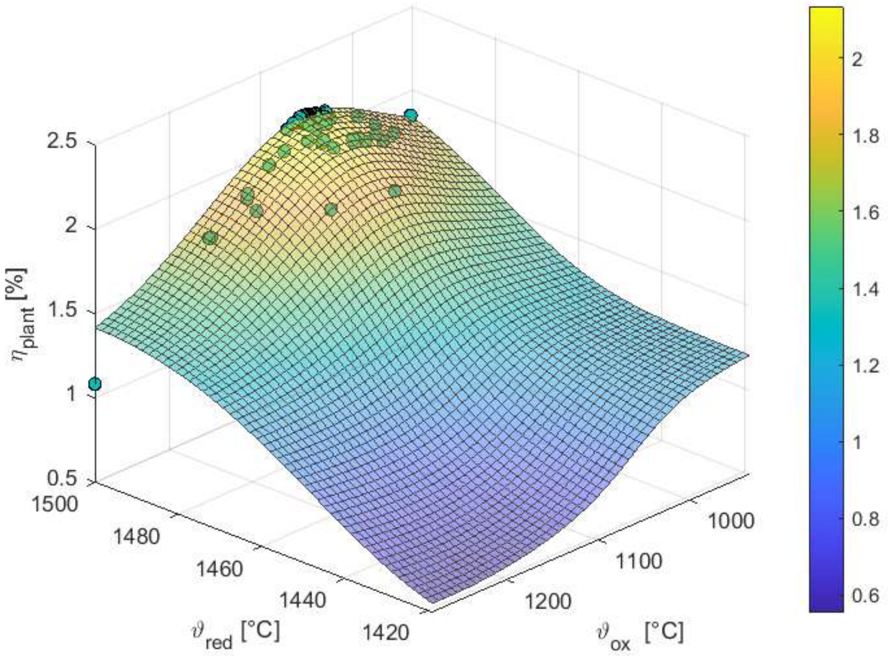
Process parameter	ϑ_{red}[°C]	ϑ_{ox}[°C]	t_{red}[s]	t_{ox}[s]	$\dot{m}_{N_2}$[kg/h]	$\dot{m}_{H_2O}$[kg/h]	η_{plant}[%]
Optimal value	1400	892.7	278.5	169.0	231.3	105.8	1.20

Optimal parameters for $\vartheta_{max} = 1500\ °C$



Contour plot of plant efficiency (for cycle times)

3D model function of plant efficiency (for temperatures)



Process parameter	ϑ_{red}[°C]	ϑ_{ox}[°C]	t_{red}[s]	t_{ox}[s]	$\dot{m}_{N_2}$[kg/h]	$\dot{m}_{H_2O}$[kg/h]	η_{plant}[%]
Optimal value	1500	1050.4	237.6	150.9	163.9	130.4	2.13

Optimal parameters for $\vartheta_{max} = 1600\ °C$ and $1700\ °C$

Process parameter	ϑ_{red}[°C]	ϑ_{ox}[°C]	t_{red}[s]	t_{ox}[s]	$\dot{m}_{N_2}$[kg/h]	$\dot{m}_{H_2O}$[kg/h]	η_{plant}[%]
Optimal value	1600	1080.4	110.0	123.6	137.5	70.8	3.92

temp-swing

vs.

isothermal

$\vartheta_{red} = \vartheta_{ox}$

Process parameter	ϑ_{red}[°C]	ϑ_{ox}[°C]	t_{red}[s]	t_{ox}[s]	$\dot{m}_{N_2}$[kg/h]	$\dot{m}_{H_2O}$[kg/h]	η_{plant}[%]
Optimal value	1600	1600	32.5	67.8	$\boxed{300.0}$	$\boxed{300}$	3.77

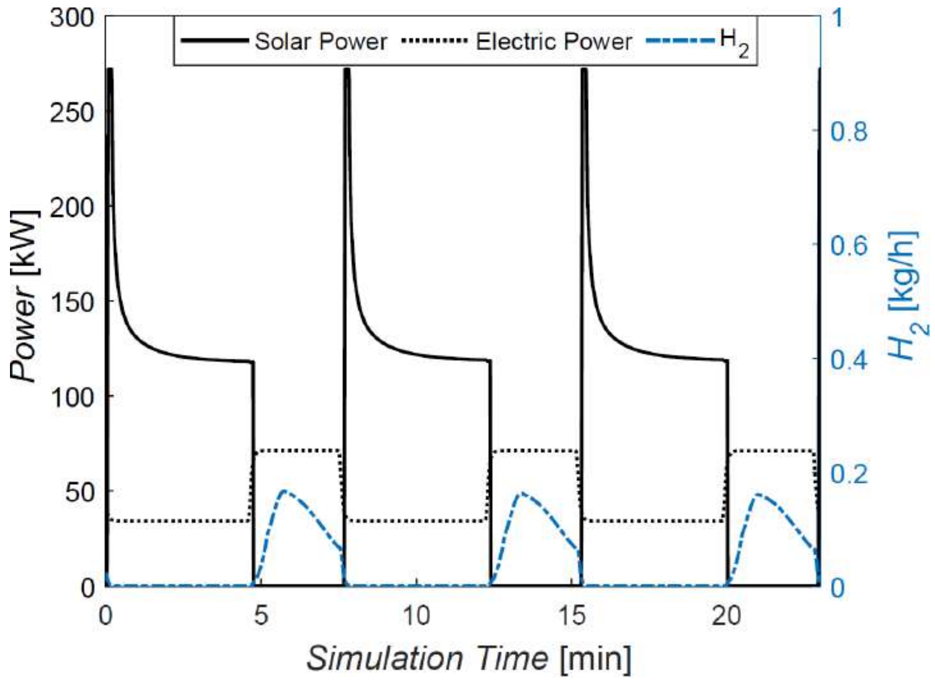
Process parameter	ϑ_{red}[°C]	ϑ_{ox}[°C]	t_{red}[s]	t_{ox}[s]	$\dot{m}_{N_2}$[kg/h]	$\dot{m}_{H_2O}$[kg/h]	η_{plant}[%]
Optimal value	1700	1139.5	93.1	90.9	144.6	126.6	5.62

Optimal operational strategy

- Reduction temperature at upper bound → the larger the better
- Optimal strategy → large and fast temperature swing
  → $\Delta\vartheta \approx 450 - 560\,°C$
  → $t_{cycle} = t_{red} + t_{ox} = 7.5 \rightarrow 3.1\,min$
  → with sufficient steam and nitrogen flow
  → $\dot{m}_{H_2O} \approx 120\,kg/h,\ \dot{m}_{N_2} \approx 140 - 230\,kg/h$
- The larger the reduction temperature…
  → …the shorter the optimal cycle
  → …the more H_2/cycle is generated

Interestingly, isothermal operation…
→ …is not much worse!
→ ... requires huge amount of steam
→ … has even shorter cycles
→ …may be superior if number of thermal cycles included in cost function

Design study for two locations



- Optimal strategy for $\vartheta_{max} = 1400\ °C$
- Multiple reactors in slightly shifted operation
  → uniform power demand
- Location considered by 12 typical daily DNI curves
- Heliostat field 10% oversized w.r.t. solar power in June
- Generated annual H_2/m^2 scales with plant efficiency

	Julich	**Tabuk**
Annual DNI $[\mathrm{kWh/m^2}]$	997.8	2946.4
Monthly average DNI $[\mathrm{kWh/m^2}]$	30-120	205-295
Heliostat field size per MW$_{th}$ $[\mathrm{m^2}]$	325.8	133.6
Average annual reactor running time $[\mathrm{h}]$	211.8	262.6
Average annual $\mathrm{H_2}$ production per reactor $[\mathrm{kg}]$	97.9	120.4
Annual produced $\mathbf{H_2}$ per heliostat area $[\mathbf{kg/m^2}]$	**0.25**	**0.76**

Conclusions

Optimal strategy for fixed-bed reactor types → large and fast temperature swings

Specific optimal process depends on

- Reactor design → heat losses, insulation
- Material limitations → maximal temperatures
- Plant layout → maximal fluid flows, valve switching times

Prototype plant efficiency for different reduction temperatures

- 1.2% for 1400 °C | 2.1% for 1500 °C | 3.9% for 1600 °C | 5.6% for 1700 °C

Efficiency can be significantly increased by reactor re-design

- Reducing radiative heat losses, e.g. by smaller aperture
- Employing high-temperature resistant material

References

1. Lampe, J., Menz, S., Akinci, K., Böhm, K., Seeger, T., Fend, T., Optimizing the operational strategy of a solar-driven reactor for thermochemical hydrogen production, *International Journal of Hydrogen Energy*, no. 47, pp. 14453–14468, 2022, doi: 10.1016/j.ijhydene.2022.02.193.
2. Menz, S., Lampe, J., Krause, J., Seeger, T., Fend, T., Holistic energy flow analysis of a solar driven thermo-chemical reactor set-up for sustainable hydrogen production, *Renewable Energy*, no. 189, pp. 1358–1374, 2022, doi: 10.1016/j.renene.2022.03.033.
3. Bulfin, B., Lowe, A.J., Keogh, K.A., Murphy, B.E., Lübben, O., Krasnikov, S.A., Shvets, I.V., Analytical model of CeO2 oxidation and reduction, *Journal of Physics and Chemistry*, no. 117, pp. 24129–24137, 2013. [Online]. Available: http: // pubs. acs. org/ doi/ abs/ 10. 1021/ jp406578z.
4. Bulfin, B., Call, F., Lange, M., Lübben, O., Sattler, C., Pitz-Paal, R. and Shvets, I. V., Thermodynamics of CeO2 Thermochemical Fuel Production, *Energy Fuels*, vol. 29, no. 2, pp. 1001–1009, 2015, doi: 10.1021/ef5019912.

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and Employment

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European Regional
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Thank you for your kind attention!

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