Modelling development of a reactor of type R2Mx for thermochemical water splitting

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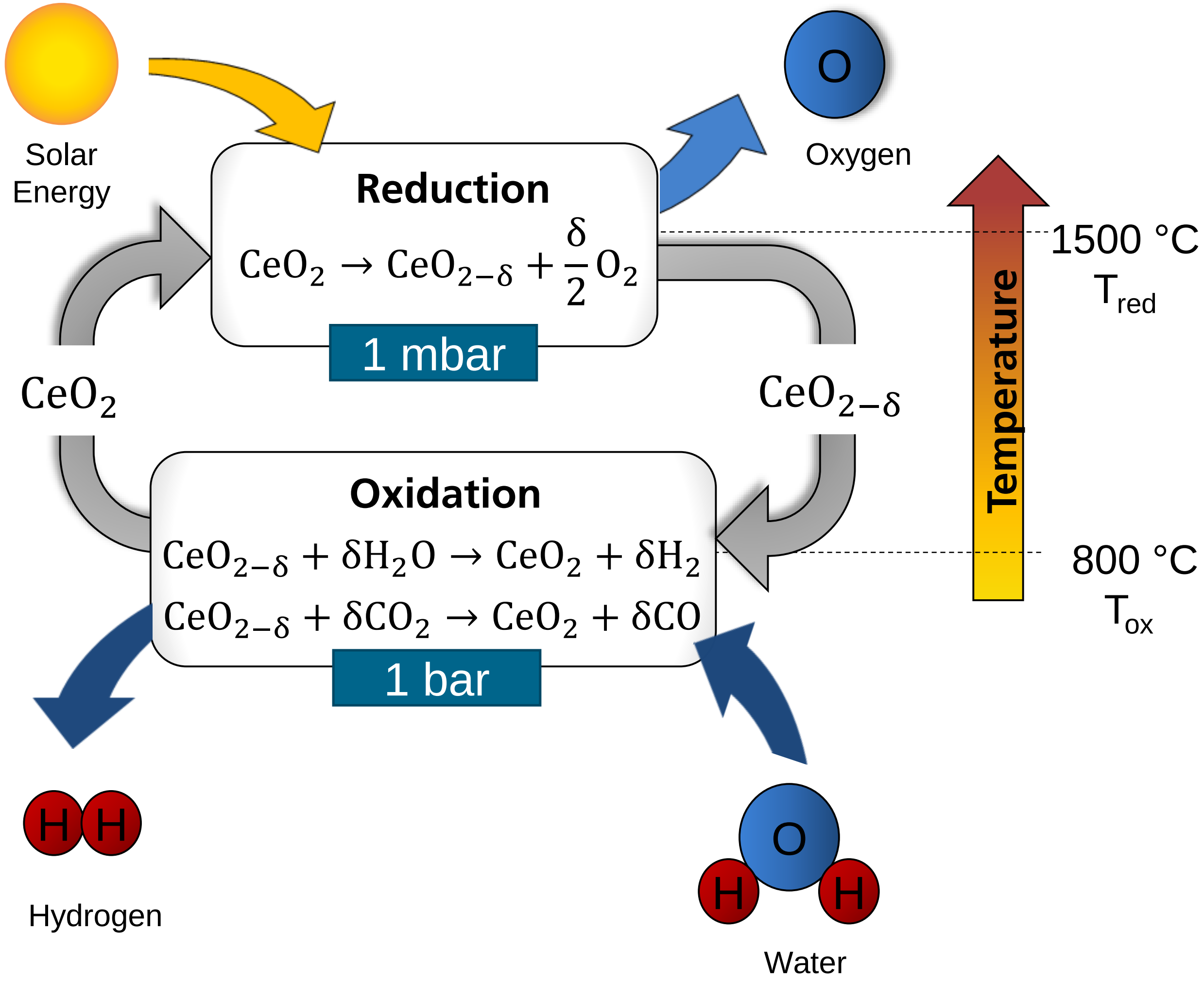
ASME
ES 2023
17th International Conference on Energy Sustainability
THE MADISON HOTEL
CONFERENCE JULY 10–12, 2023

Two-step thermochemical redox cycles

Chemical reaction and state-of-the-art reactor technology



Solar Energy

Oxygen

O

Reduction

$$CeO_2 \rightarrow CeO_{2-\delta} + \frac{\delta}{2} O_2$$

1 mbar

CeO_2

$CeO_{2-\delta}$

Oxidation

$$CeO_{2-\delta} + \delta H_2O \rightarrow CeO_2 + \delta H_2$$

$$CeO_{2-\delta} + \delta CO_2 \rightarrow CeO_2 + \delta CO$$

1 bar

Temperature

1500 °C

T_{red}

800 °C

T_{ox}

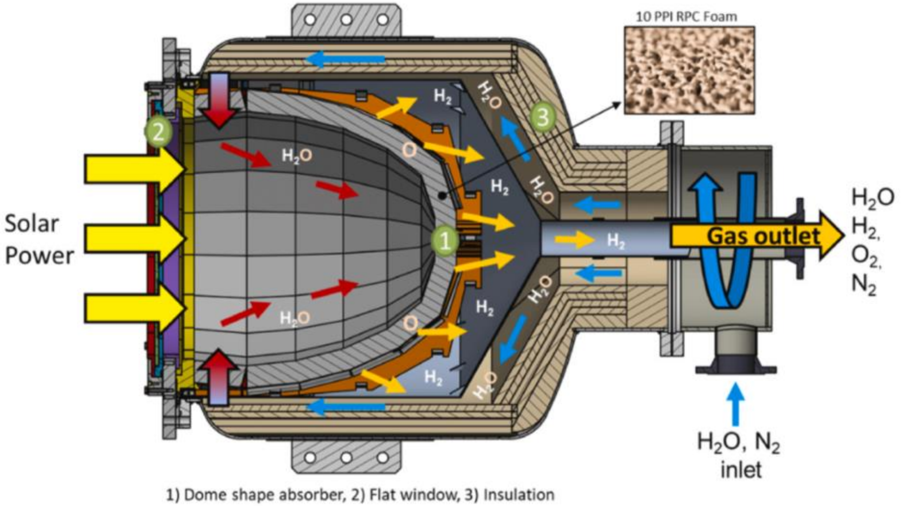
H H

Hydrogen

O

H H

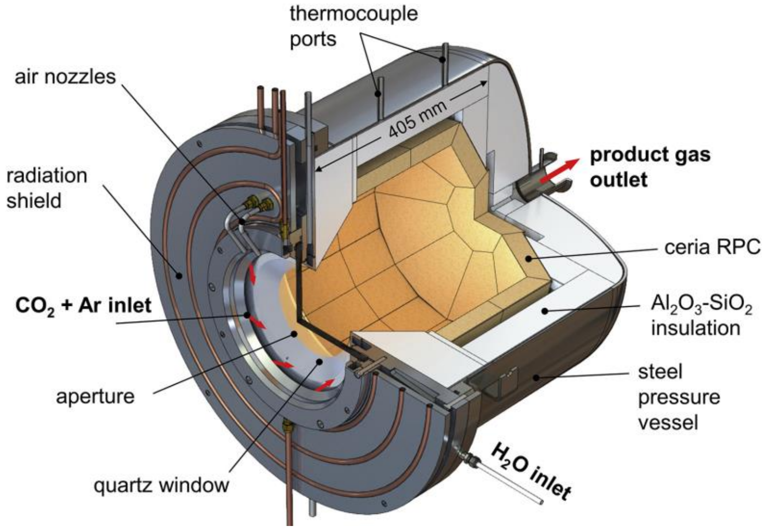
Water



1) Dome shape absorber, 2) Flat window, 3) Insulation

HYDROSOL & ASTOR projects

Thanda, V. et al. *Renewable Energy*, 2022



https://www.sun-to-liquid.eu/

Zoller, S. et al. *Joule*, 2022

Characteristics of a next generation receiver-reactor

Receiver-reactor wish list

High efficiency

Modular system

Good scalability

Strategies

- Solid-solid heat recovery
- Avoid cyclic heating of inert reactor components
- Continous reduction reaction

Characteristics of a next generation receiver-reactor

Receiver-reactor wish list

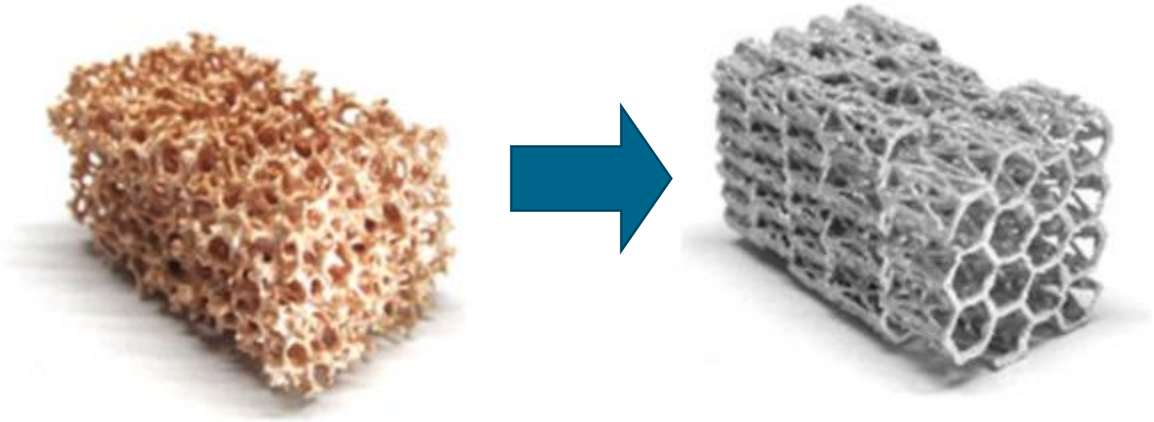
High efficiency

Modular system

Good scalability

- Defined component interfaces
- Fast and simultaneous development of reactor components

- Uncomplicated adaptation to new redox material



Images adapted from Hoes. M et al. *Energy Technology*, 2018

Characteristics of a next generation receiver-reactor
Receiver-reactor wish list

High efficiency

Modular system

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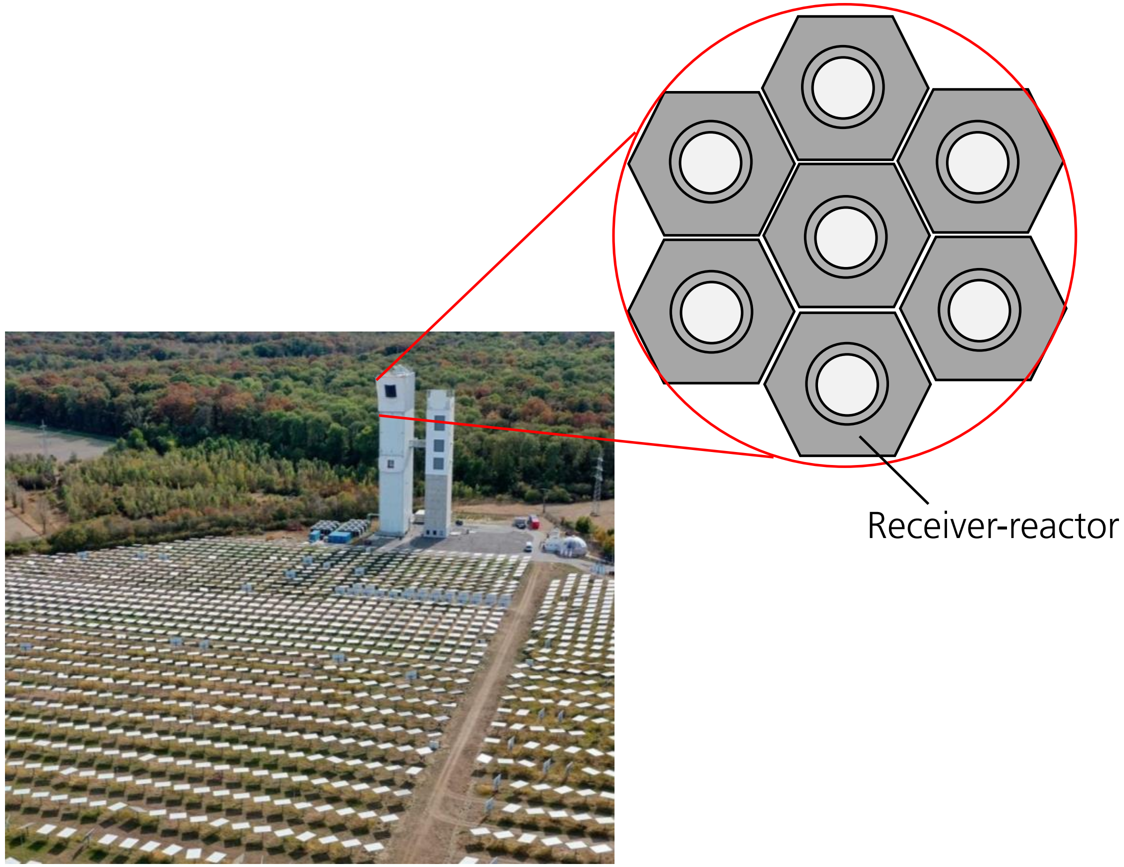
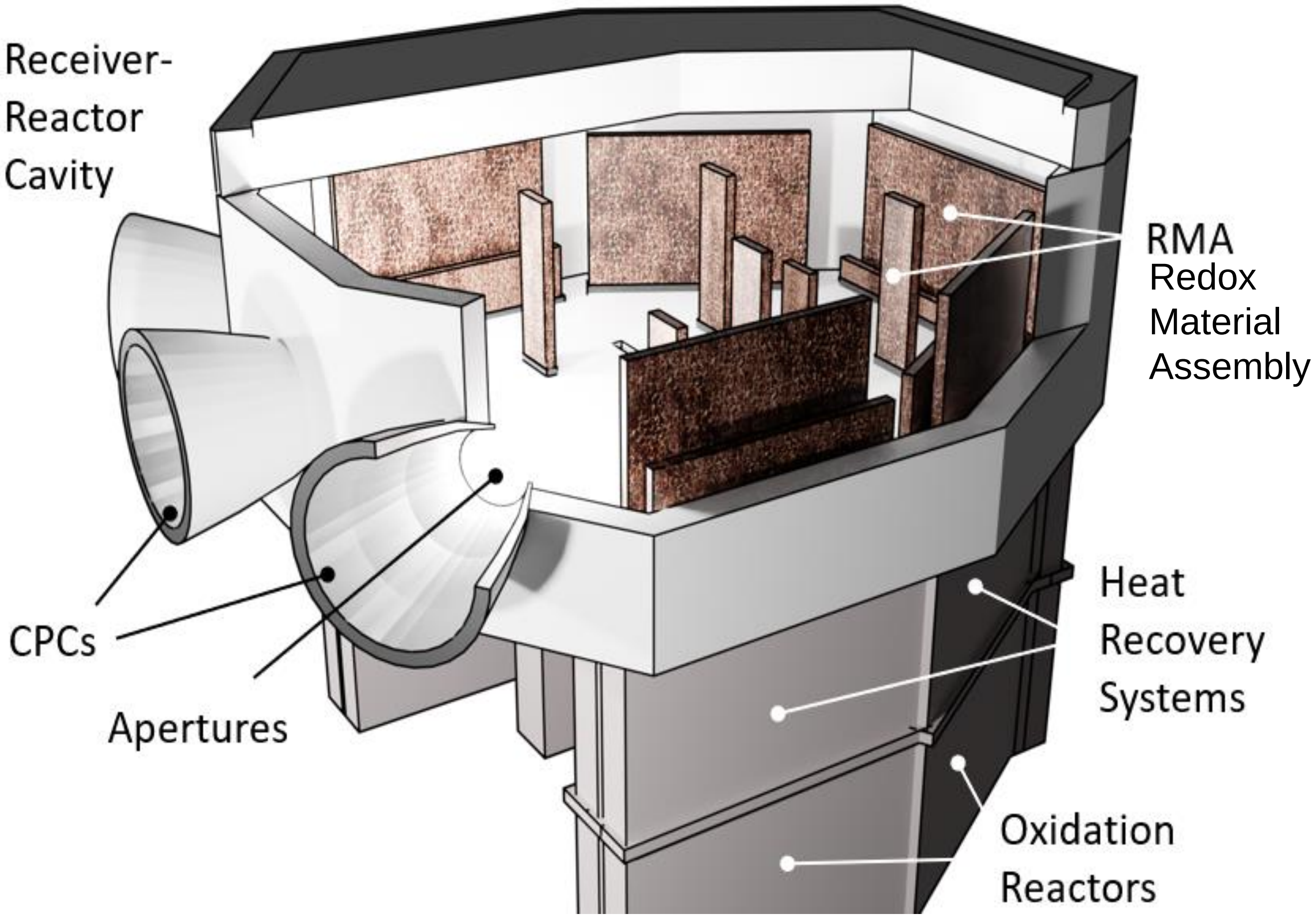


- Avoid batched array operation

R2Mx receiver-reactor

Receiver-reactor cavity system with multiple mobile redox units



MW scale vision of the R2Mx receiver-reactor

Reactor features:

R2Mx	State-of-the-art
Separated reduction and oxidation zones	Only one reaction zone
Continuous on-sun operation	Batch operation
Movable redox material	Stationary redox material
Linear transportation system	No transportation system
Solid-solid heat recovery	No solid-solid heat recovery

Theoretical efficiency 12-14%

- Simplified model without optimizations or heat recovery

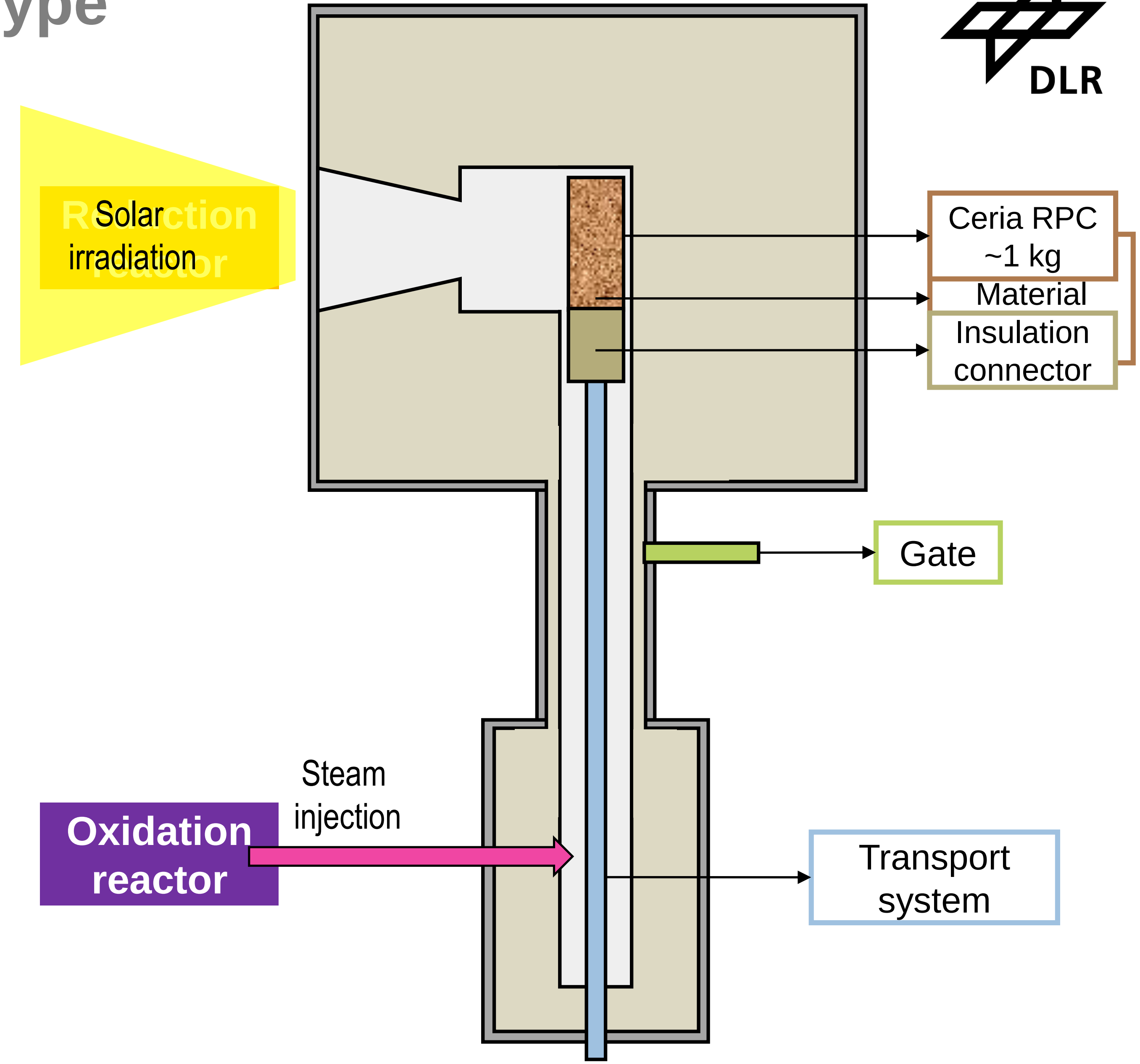
Brendelberger, S.; Holzemer-Zerhussen, P.; Vega Puga E. et al. *Solar Energy,* 2022

R2Mx receiver-reactor prototype

- Experimental demonstration of R2Mx working principle at DLR

Features included:

- Pressure sealing between reactors at high temperatures (1500 °C) and vacuum (1 mbar)
- 2 distinct reaction zones
- Transport of hot redox material (T~1500°C) in vacuum

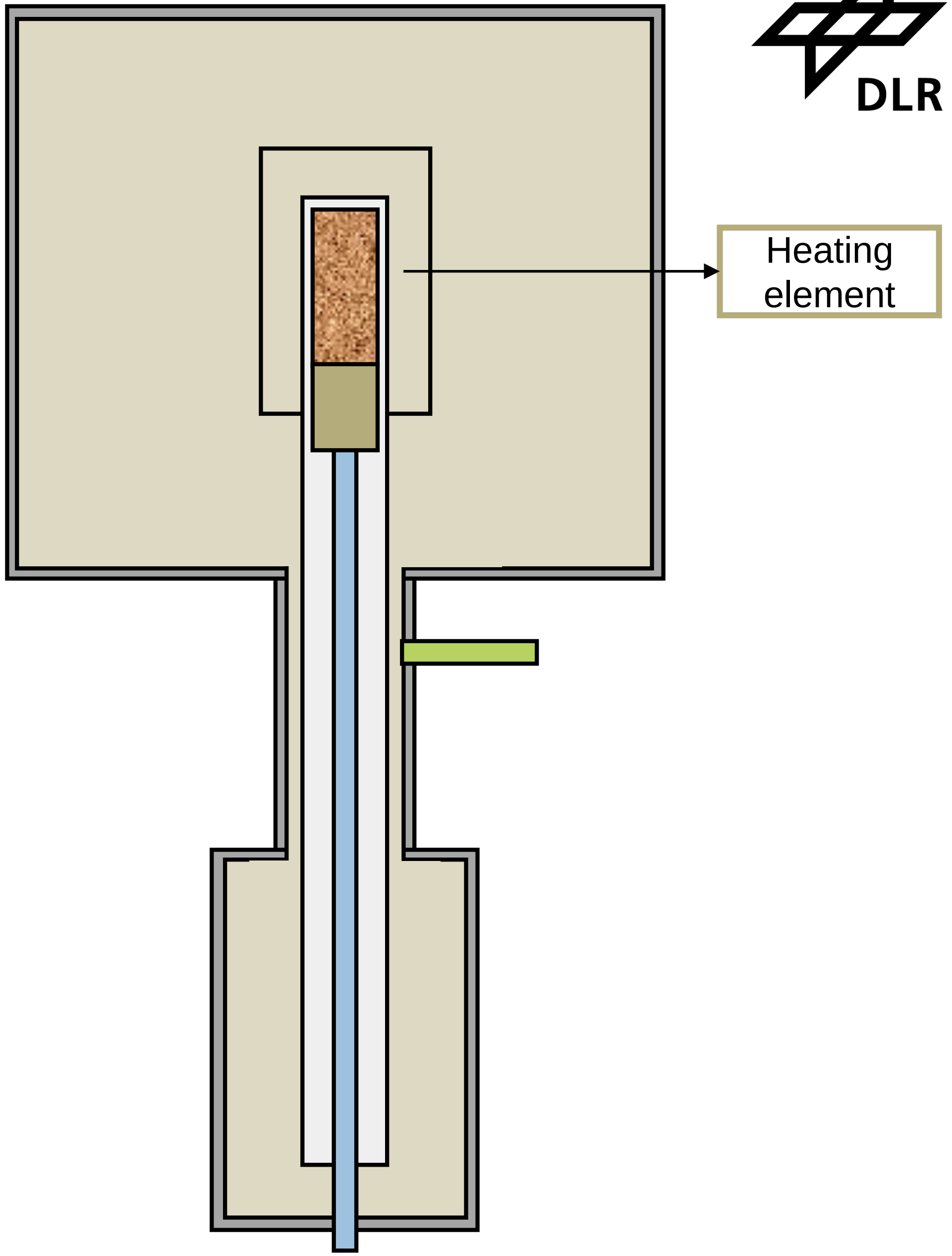


R2Mx test stand FE simulation

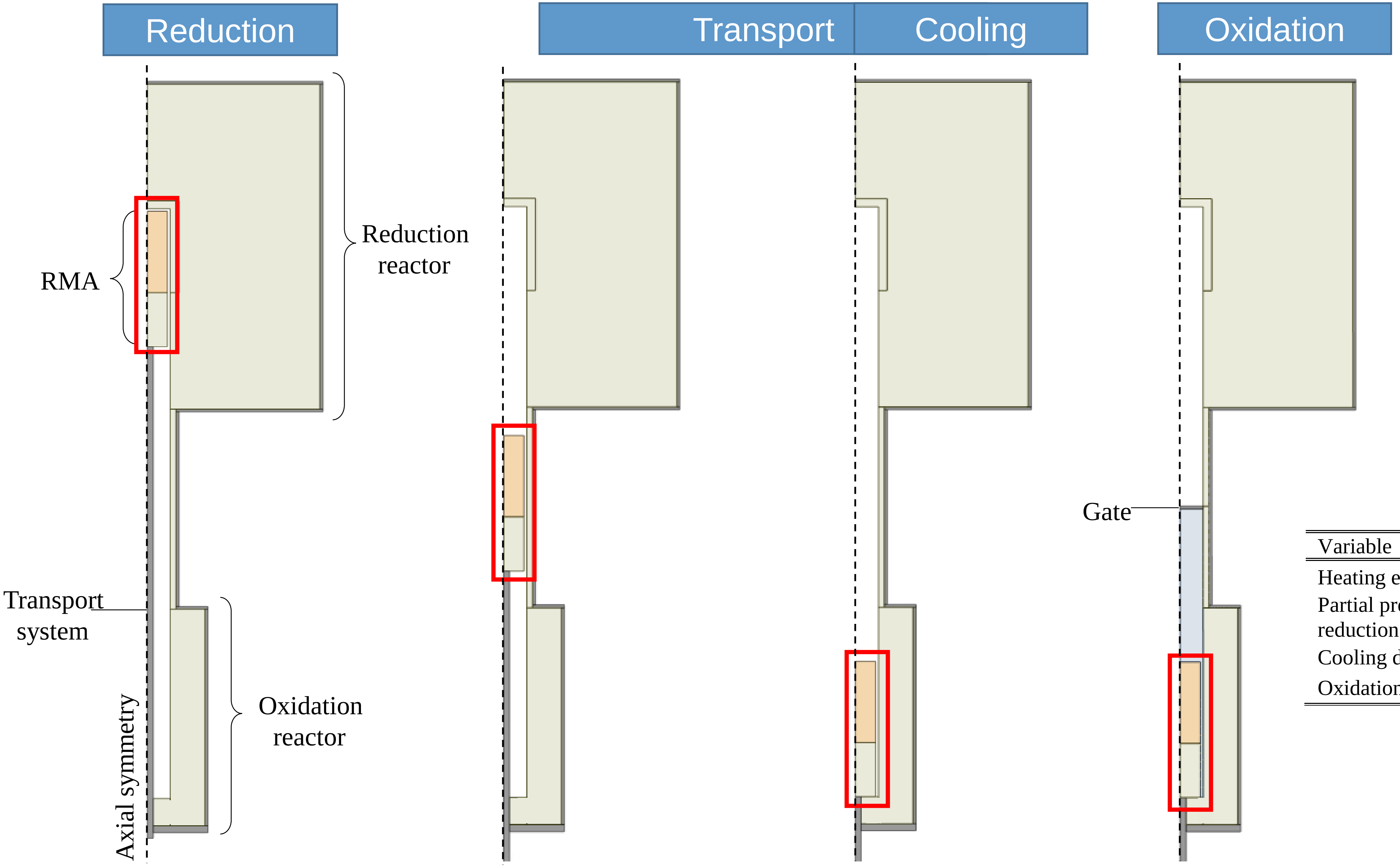
Goals of the study:

- ✓ Understanding of temperature distribution and loads during cyclic operation
- ✓ Derivation of reasonable duration of reaction steps
- ✓ Proof initial material selection
- ✓ Sizing of components (electrical heater and vacuum pump)

- 2D axisymmetric transient heat transfer simulation in ANSYS Mechanical
- Includes chemical reaction and internal radiation heat transfer in the porous redox material
- Simulates 5 consecutive cycles (reduction, transport, cooling, oxidation and transport)

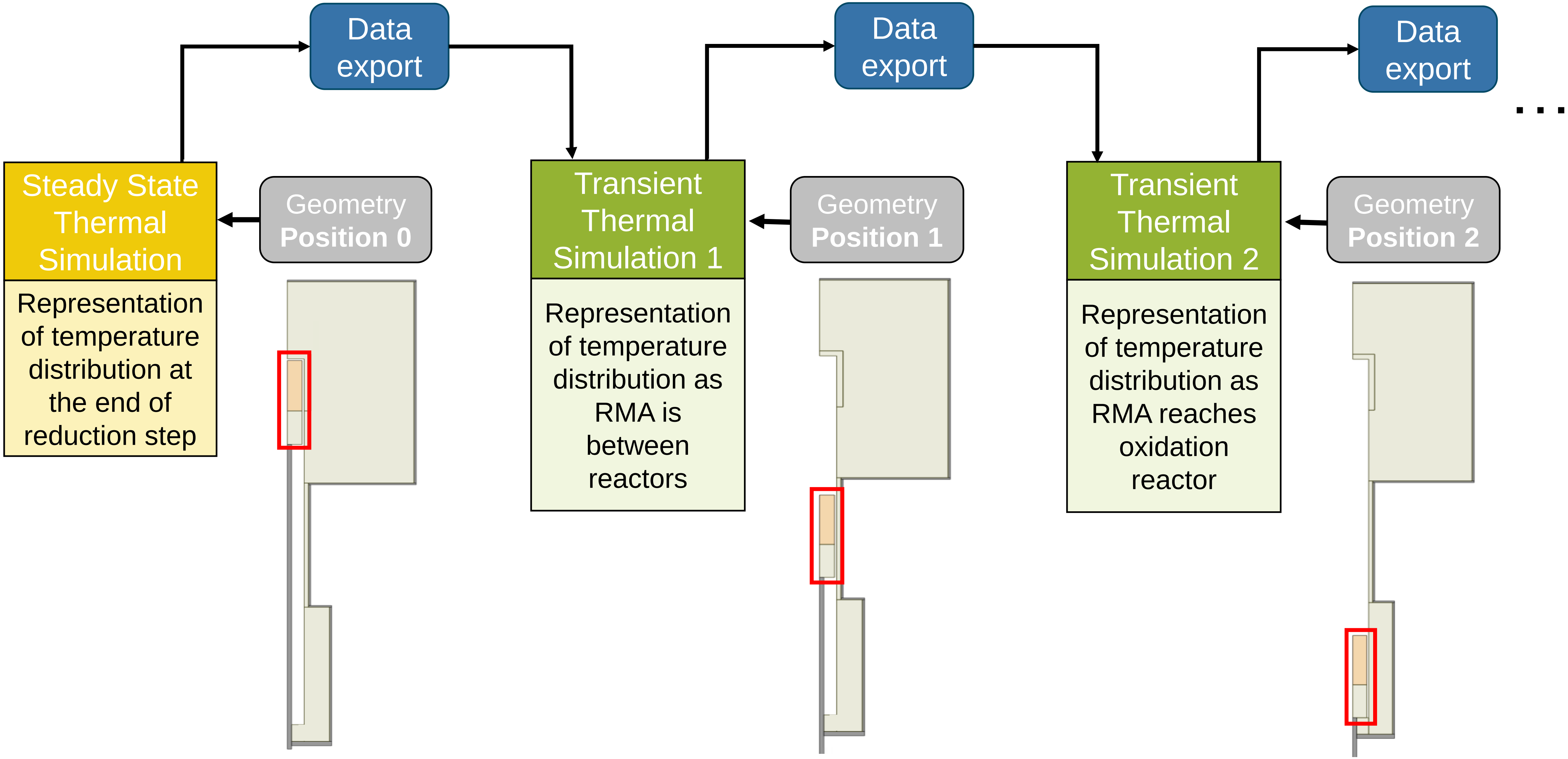


Geometries



Variable	Value
Heating element temperature	1500 °C
Partial pressure of oxygen in reduction reactor	1 mbar
Cooling duration	5.5 min
Oxidation duration	8 min

Simulation workflow



Steady State Thermal Simulation

Representation of temperature distribution at the end of reduction step

Data export

Geometry **Position 0**

Transient Thermal Simulation 1

Representation of temperature distribution as RMA is between reactors

Data export

Geometry **Position 1**

Transient Thermal Simulation 2

Representation of temperature distribution as RMA reaches oxidation reactor

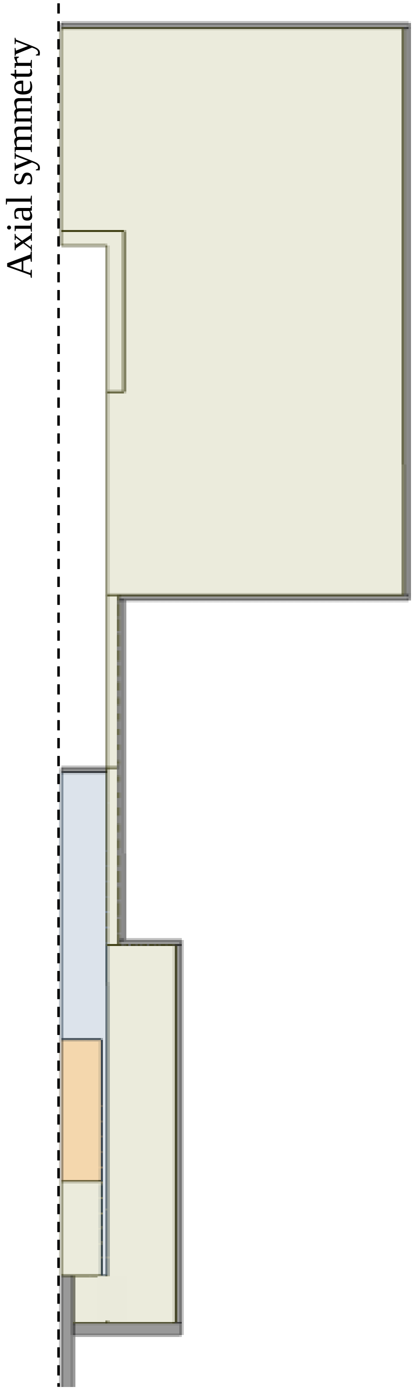
Data export

Geometry **Position 2**

…

Simulation workflow (Oxidation)

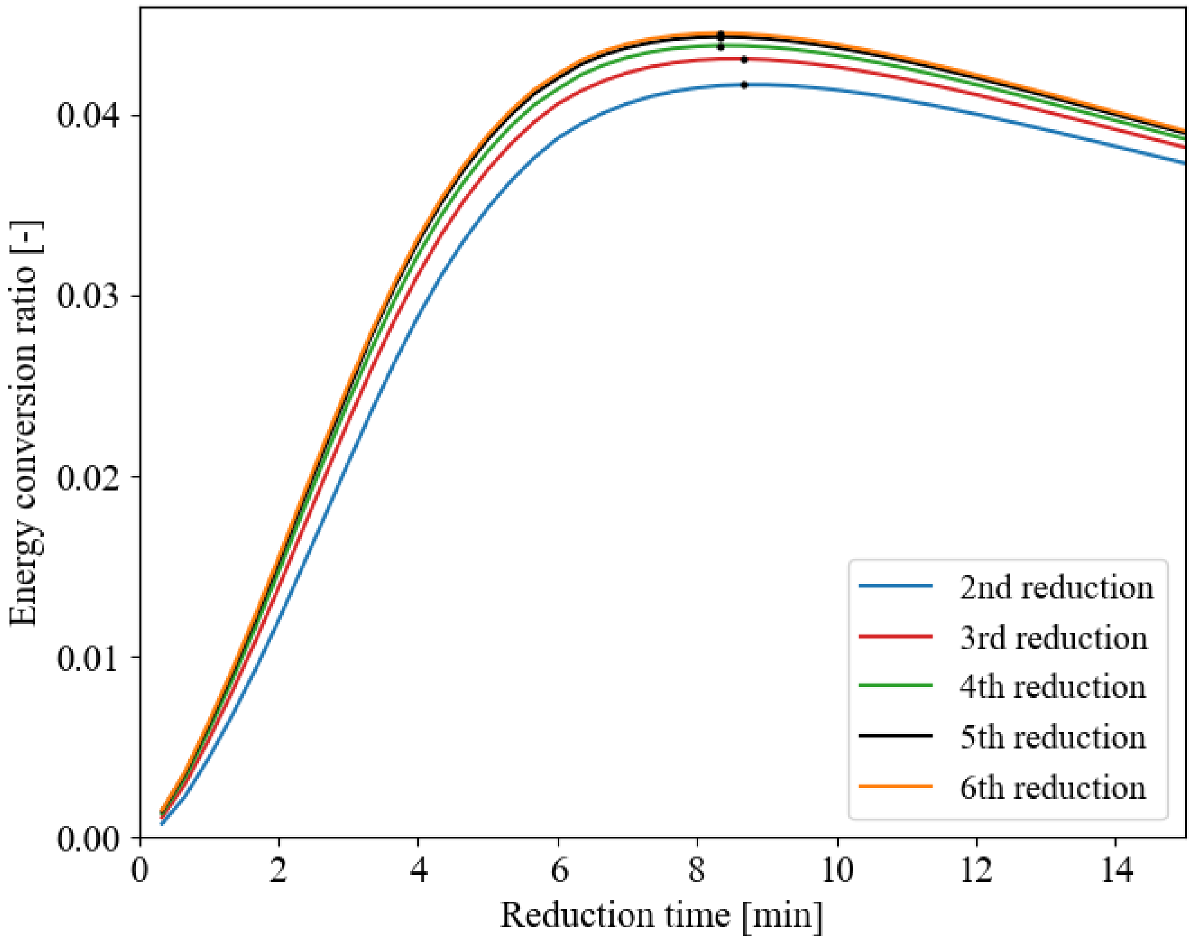
- In reality, steam flows through the oxidation reactor for ~8min
- The effect of fluid exchange approximated by a complete replacement of the fluid with a cold steam several (10) times
- Simulated by a series of transient simulations coupled to each other
- The solution from a previous simulation is used as initial condition for the next



Base case results
Reduction step duration

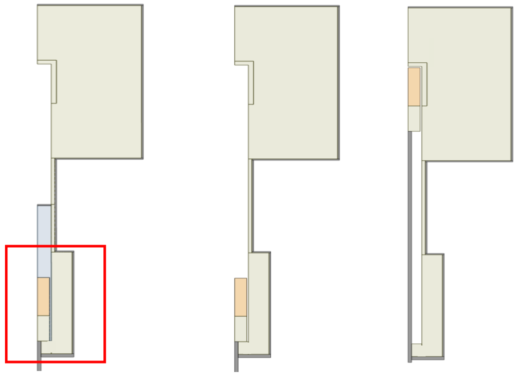
- When the maximum energy conversion ratio (r_{econv}) is achieved, the reduction is stopped

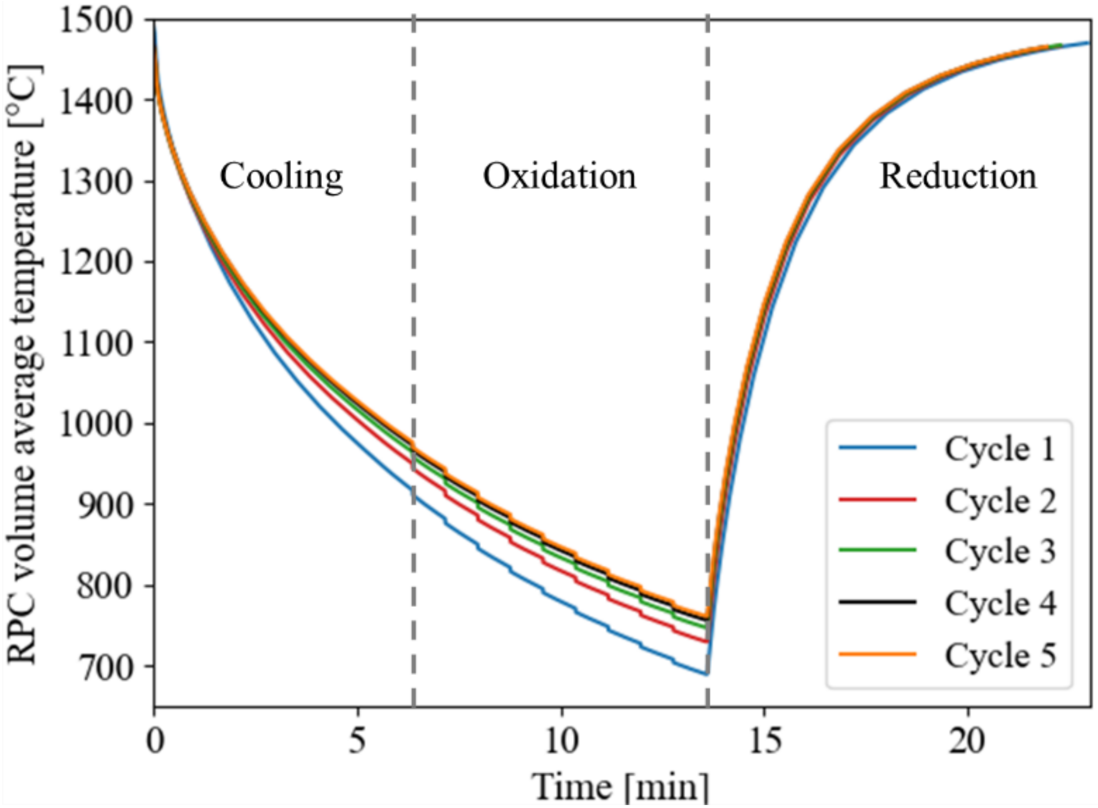
$$r_{\text{econv}} = \frac{n_{\text{H}_2}\text{HHV}_{\text{H}_2}}{Q_{\text{Heating element}}}$$

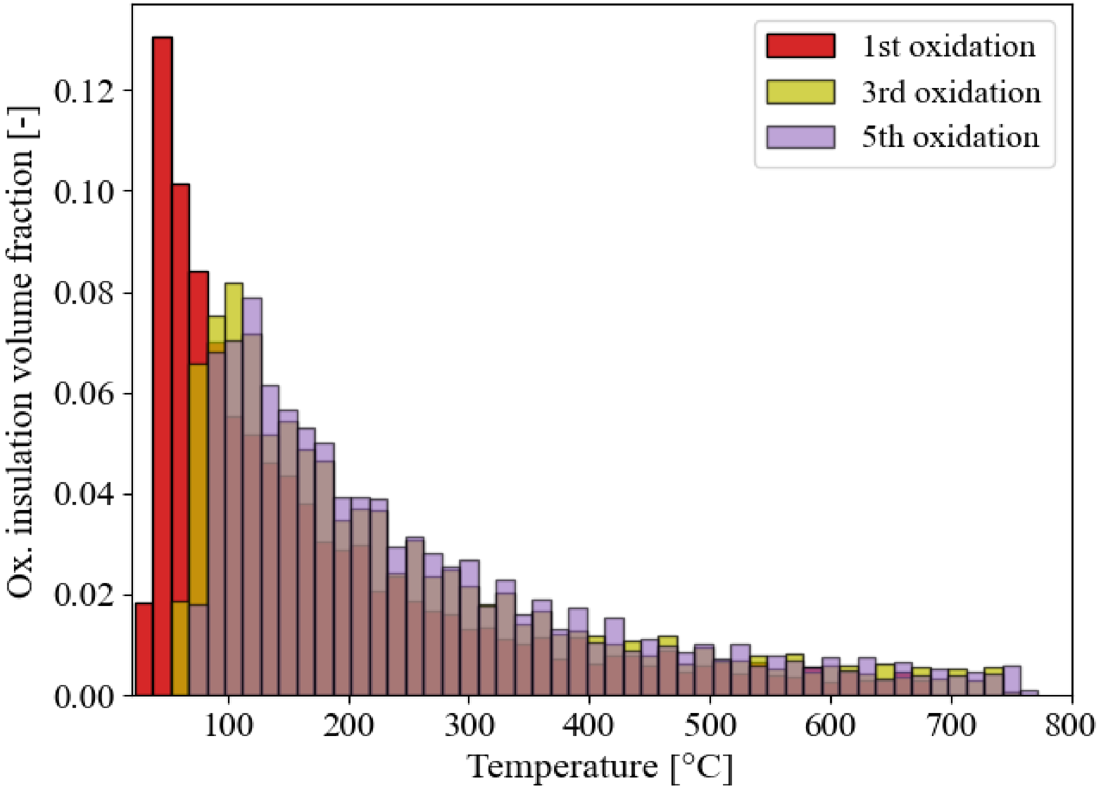


Duration of reduction step remains fairly constant throughout the cycles

Base case results
Temperature distribution







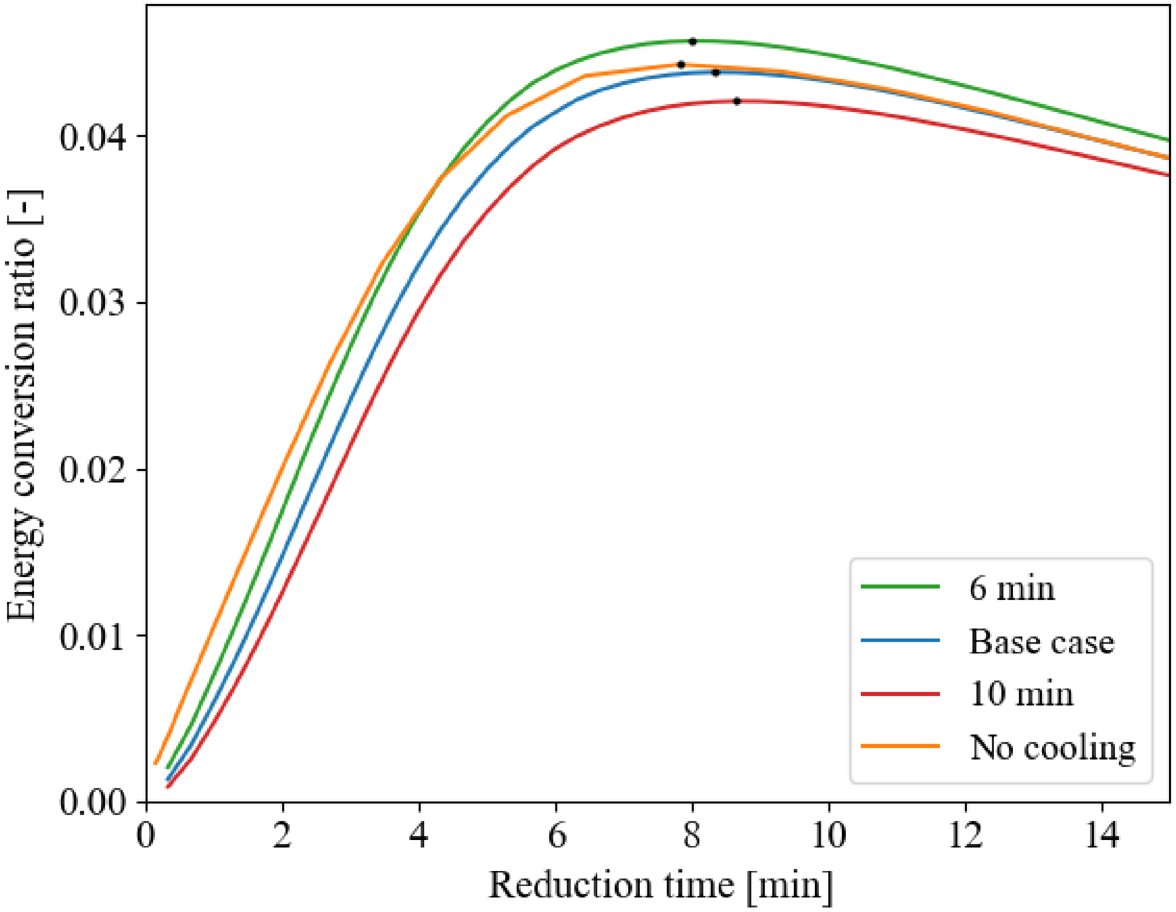
Converged min vol. avg. T_{RPC} ≈ 760°C after 10 cycles

Parametric analysis of operation modes
Changing oxidation length

Reduction step duration

- When the maximum energy conversion ratio (r_{econv}) is achieved, the reduction is stopped

$$r_{\mathrm{econv}} = \frac{n_{\mathrm{H_2}} \mathrm{HHV}_{\mathrm{H_2}}}{Q_{\mathrm{Heating\ element}}}$$



Duration of reduction step remains fairly constant regardless of operation mode

Summary and Outlook

- ✓ **Development of model** including **RMA movement** and **cyclic operation**
  - ✓ Derived **approximate step durations** for reasonable operation
  - ✓ Estimated **maximum** expected **temperatures of components**
  - ✓ Evaluated **material selection**
  - ✓ Performed **component** (heater and vacuum pump) **sizing**

- 🔍 **Start of experimental campaign** of test stand at the **end of 2023**

Impressum

Federal Ministry
for Economic Affairs
and Climate Action

DLR

Topic: **Modelling development of a receiver-reactor of type R2Mx for thermochemical water splitting**

Date: 12.07.2023

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Institute: Future Fuels

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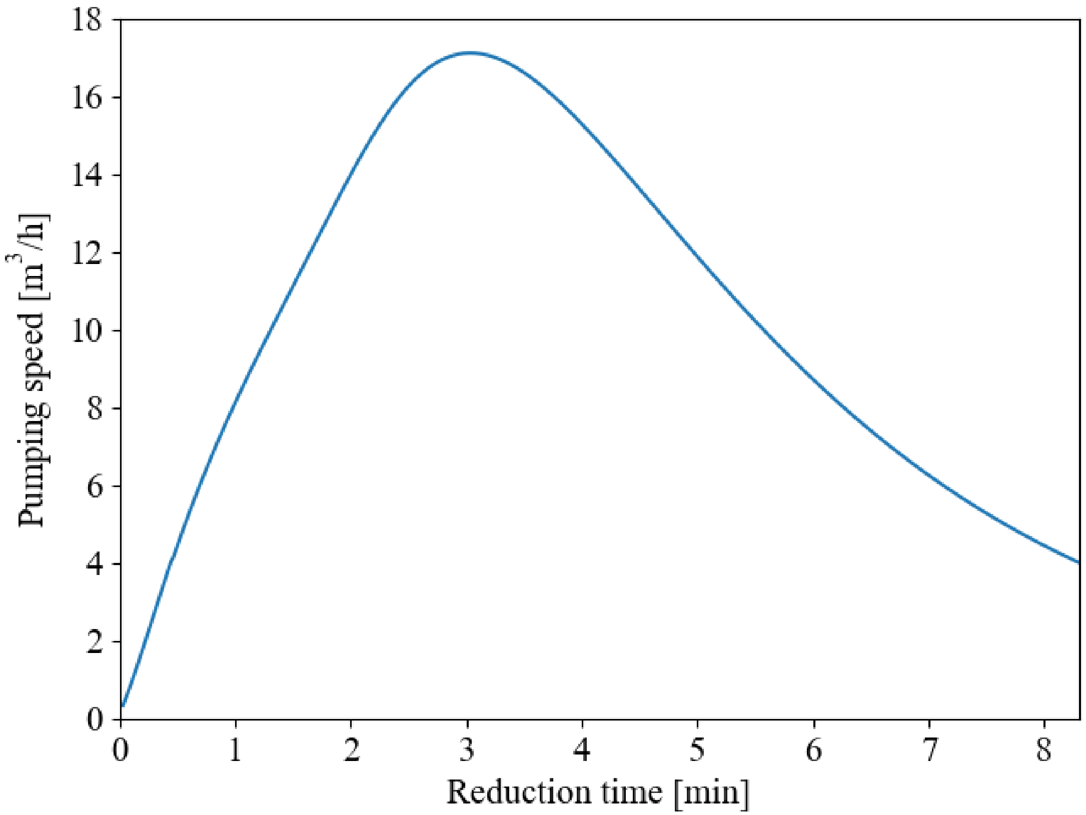
BACK UP SLIDES

Base case results

Component sizing

- ✓ **Heating unit** of the reduction reactor = **1450 W**
- ✓ Vacuum pump's **maximum pumping speed** = **17 m^3/h**



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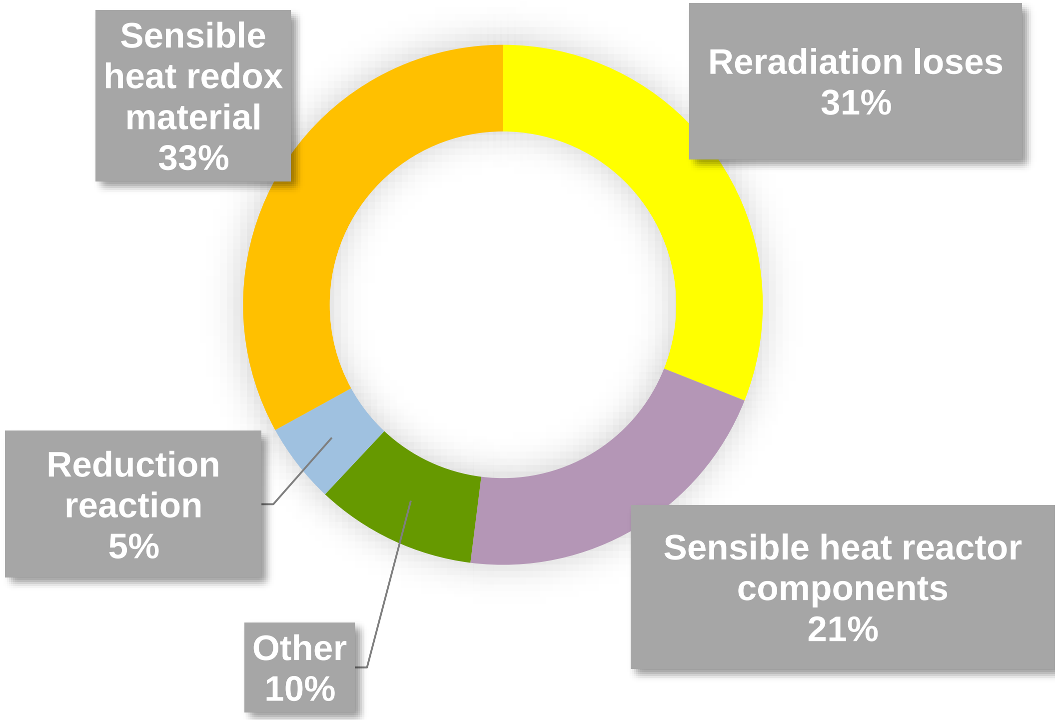
Receiver-reactor wish list

High efficiency

Modular system

Good scalability

Energy demand during reduction [1]

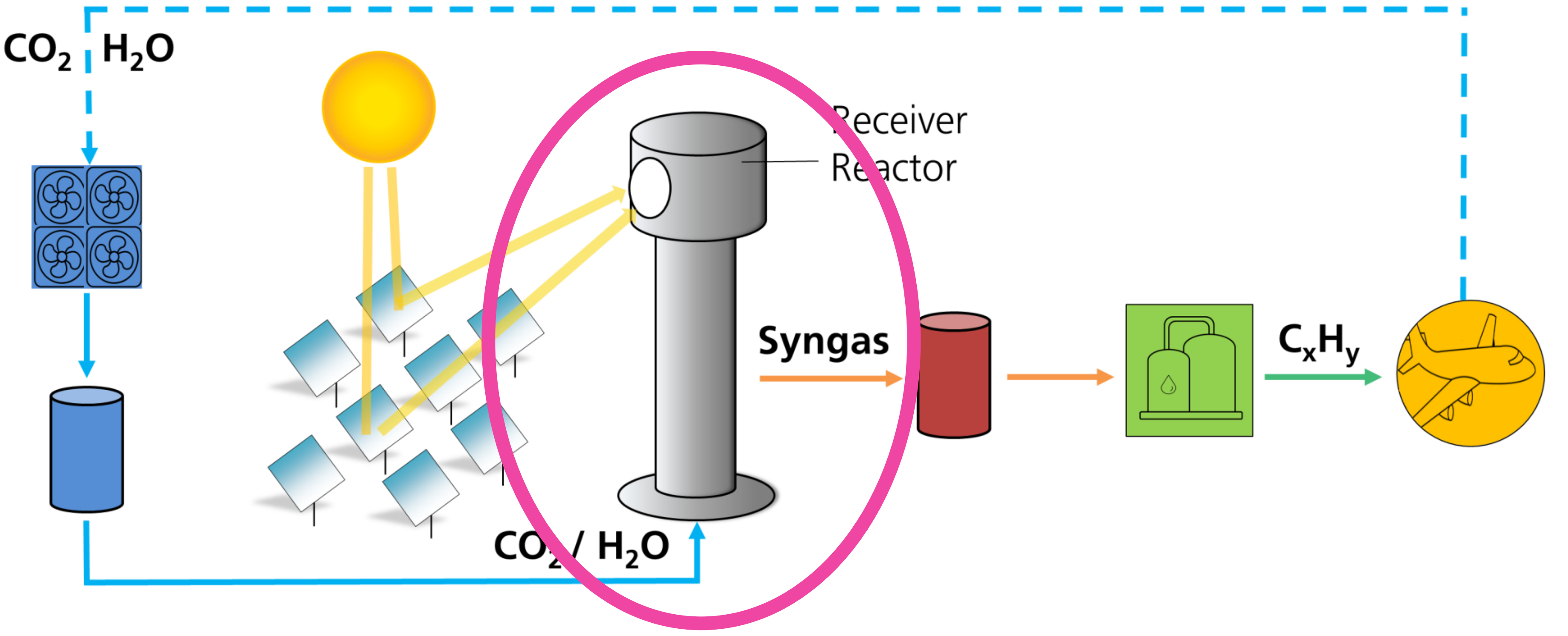


[1] Data from Zoller, S. et al. *Journal of Solar Energy Engineering*, 2018

Motivation

Production of fuels and chemicals

Solar pathway for sustainable aviation fuel



Direct Air Capture | Solar Concentration | Thermo-chemistry | Gas Storage | Fischer - Tropsch | Combustion

Cavity receiver-reactor – Challenges

Limited efficiency improvement of scaled-up system

- Relates to usage of redox material – mostly the surface is relevant

Zoller et al. (2019)

No solid-solid heat recovery

- Solid-solid heat recovery difficult to implement
- Use of a heat transfer fluid poses an engineering challenge

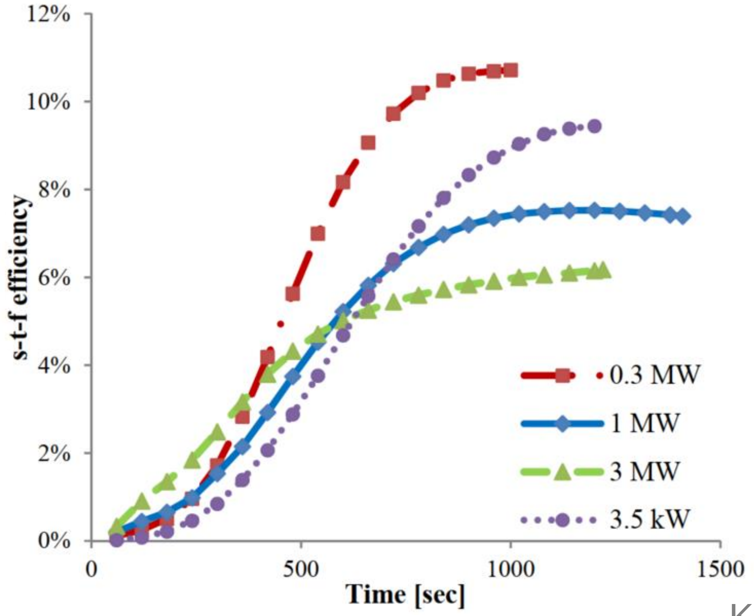
Brendelberger et al. (2019)

Receiver-reactor array efficiency penalty

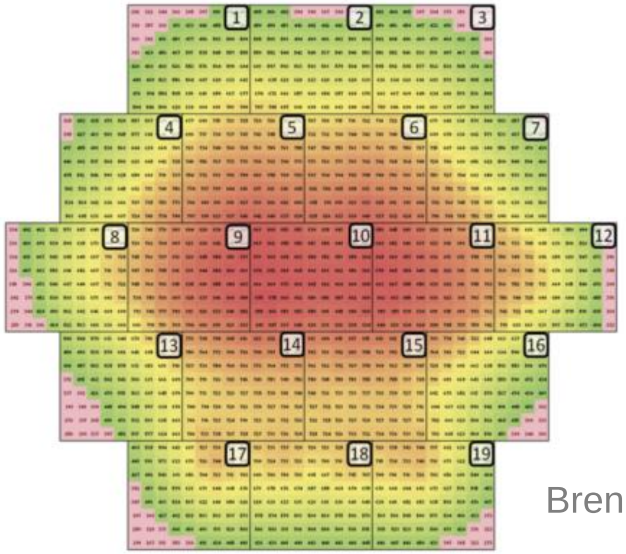
- Inhomogeneous flux distribution
- Limited off-design performance of receiver-reactors

Batch operation

- Cyclic heating and cooling of reactor components



Kyrimis et al. (2019)



Brendelberger et al. (2020)

Flux distribution of a 10 MW receiver-reactor array

R2Mx – 1st Numerical Assessment

Theoretical efficiency 12-14%

- Simplified model without optimizations or heat recovery

Solid-solid heat recovery

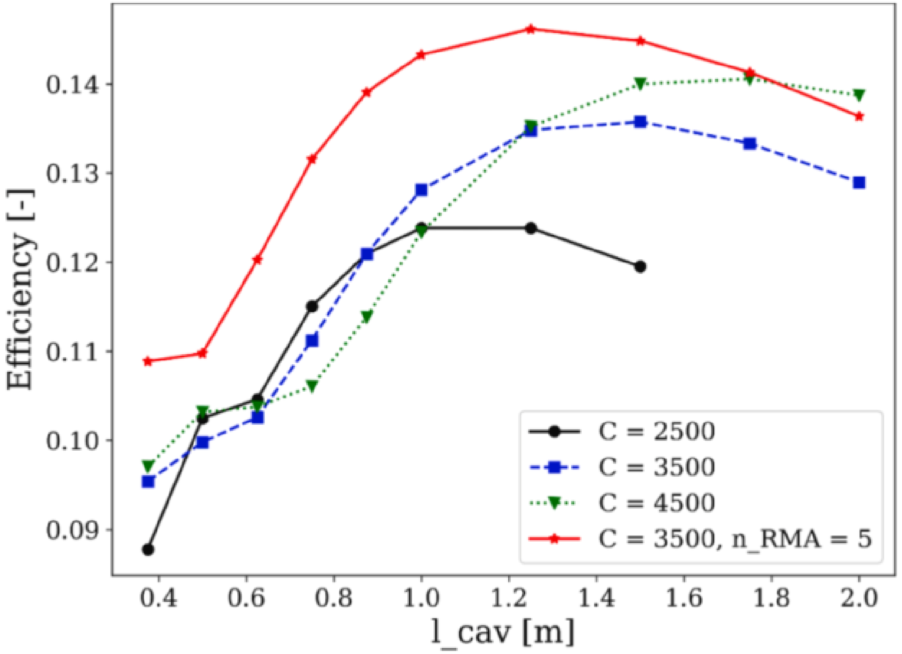
- Predicted recovery rate of ~15%

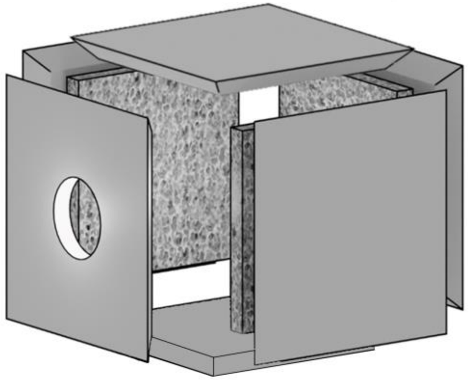
Independent RMA operation

- Good part-load operation and further optimization potential

Improved solar field efficiency

- Continous on-sun operation





Brendelberger, S.; Holzemer-Zerhussen, P.; Vega Puga E. et al. *Solar Energy,* 2022

Governing Equation

Heat conduction through a solid (3D) given by:

$$k\left(\frac{\partial^2 T}{\partial x^2}+\frac{\partial^2 T}{\partial y^2}+\frac{\partial^2 T}{\partial z^2}\right)+q=\rho c\frac{\partial T}{\partial t}$$

Rate of heat conduction

Rate of heat flux/convection/ radiation/internal heat generation inside the volume

Rate of energy storage inside the volume

- Boundary Conditions:

Convection to ambient

$$q_{\text{conv}} = h\,A\,(T_s - T_{amb})$$

Radiation to ambient

$$q_{\text{rad\_amb}} = \varepsilon_s\,\sigma\,({T_s}^4 - {T_{amb}}^4)$$

Radiation between surfaces

$$q_{\text{rad\_out,s}} = \varepsilon_s\,\sigma\,{T_s}^4 + \rho_s\sum_{j=1}^{N} F_{sj}\,q_{\text{rad\_out,j}}$$

k = Thermal conductivity (in $W/K\cdot m$)

t = Time

T = Temperature (in K)

ρ = Density of the material (in kg/m^3)

c = Specific heat of the material (in $J/kg\cdot K$)

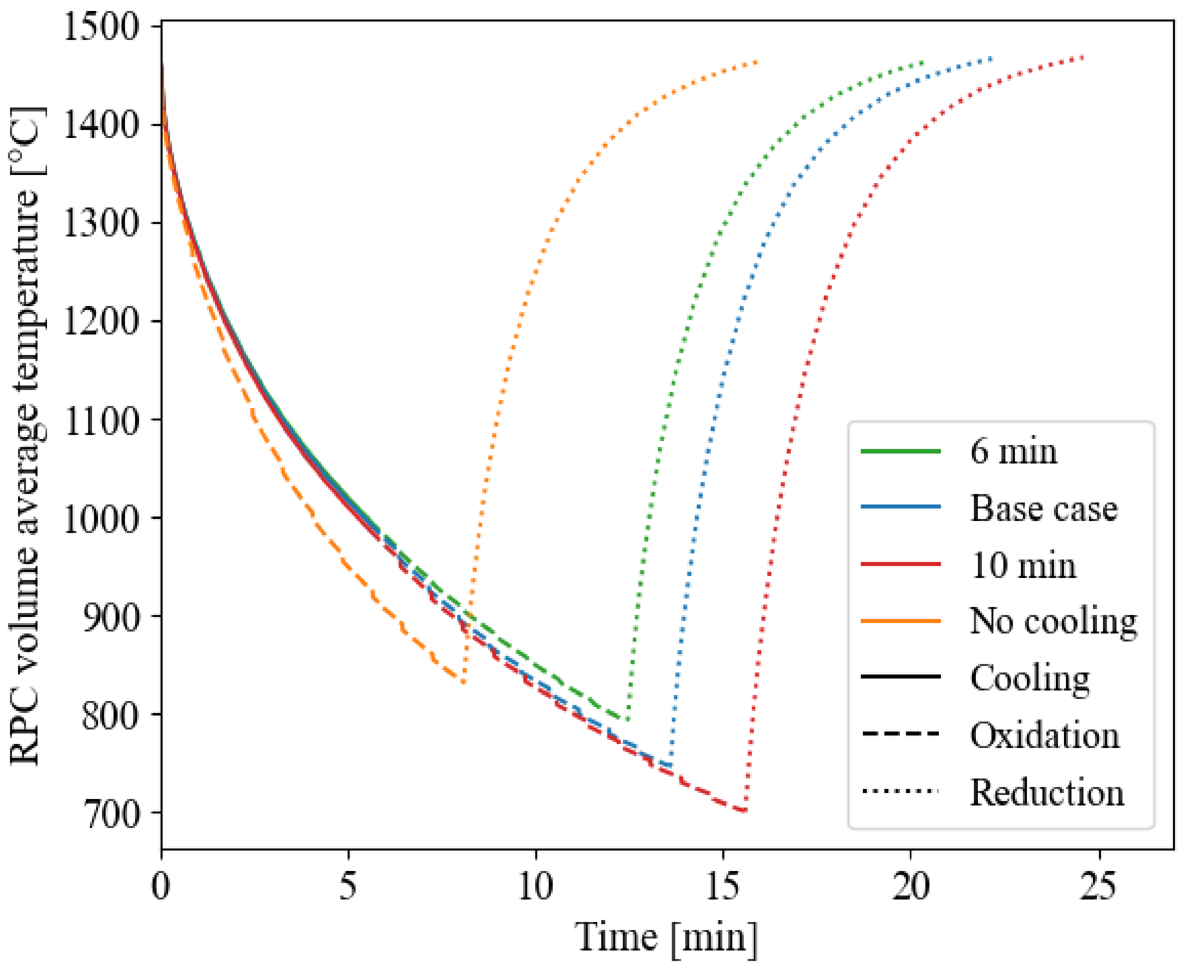
h = film coefficient (in W/K m^2)

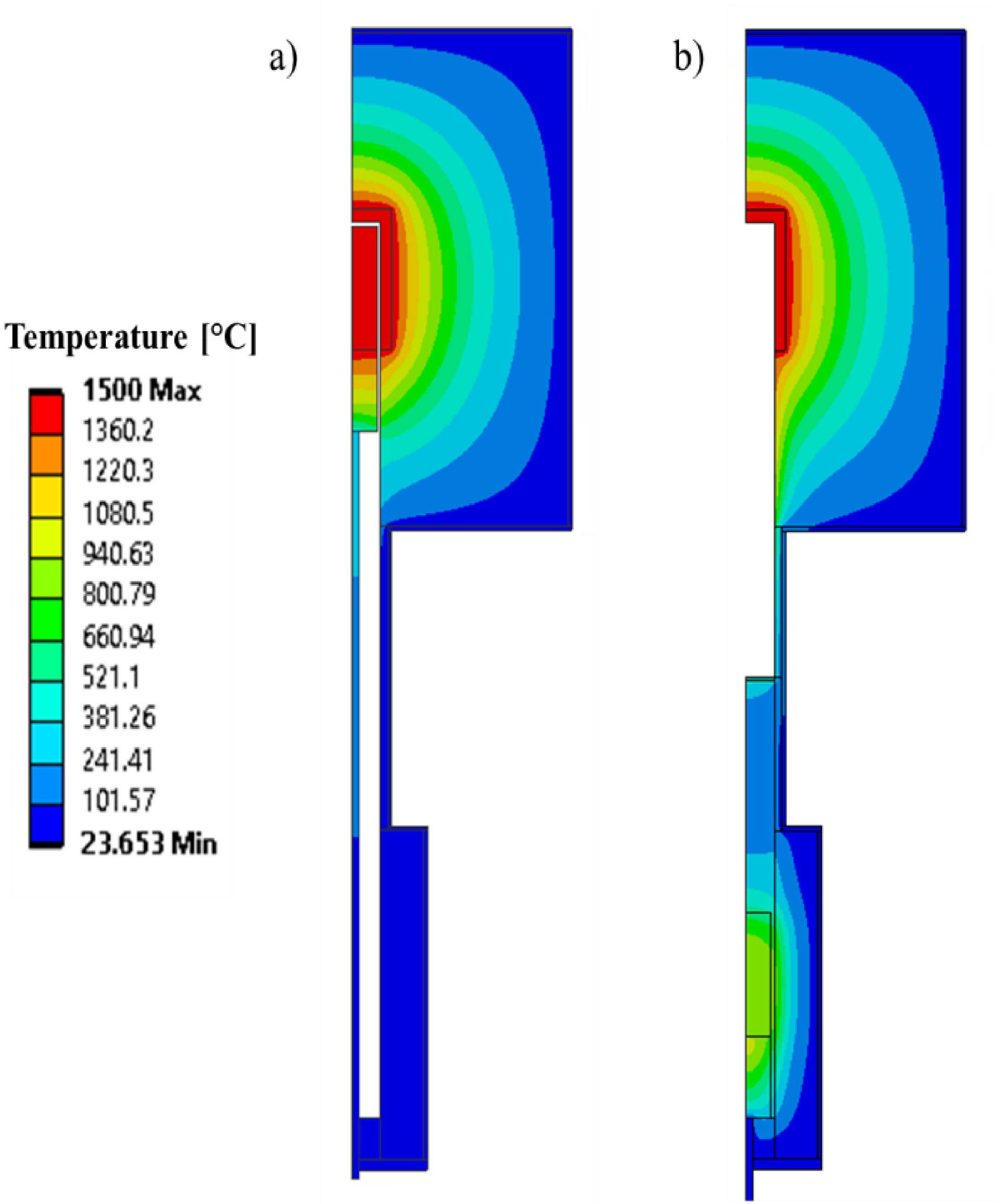
A = surface area (in m^2)

ε_s = Material emissivity

F_{sj} = View factor from surface s to surface j

Parametric analysis of aperation modes
Changing oxidation lenght




a)
b)
Temperature [°C]
1500 Max
1360.2
1220.3
1080.5
940.63
800.79
660.94
521.1
381.26
241.41
101.57
23.653 Min