2nd EU-SOLARIS DOCTORAL COLLOQUIUM and 1st EU-SOLARIS SUMMER SCHOOL

Almería, Spain, June 2nd – 4th 2025

Development of a solar-thermochemical reactor for sustainable production of high-purity nitrogen using concentrated solar power

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Supervisor: Dr. Lena Klaas

Funded by the European Union

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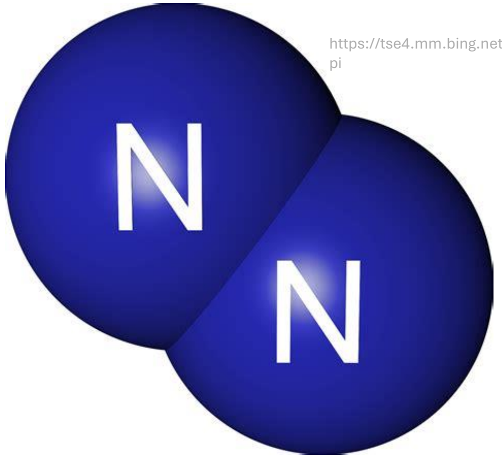
Agenda



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DLR Project Sesam, Final presentation

Katrin Klingel

04.06.2025

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Relevance of ammonia

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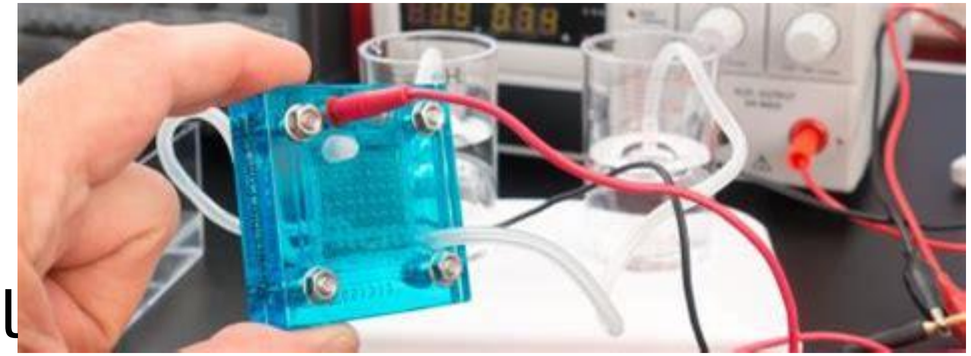
Fuel cell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Relevance of Nitrogen

- Ammonia is conventionally produced by hydrogen from reforming of natural gases and nitrogen from air
  - Significant amount of greenhouse gases
  - Decarbonisation!
- Alternative: production via Haber-Bosch process from hydrogen and nitrogen
  - High purities of <10ppm remaining oxygen in nitrogen are necessary [1]
  - Green hydrogen & green nitrogen are required

[1] Bulfin, B.; Buttsworth, L.; Lidor, A.; Steinfeld, A. (2021): High-purity nitrogen production from air by pressure swing adsorption combined with SrFeO 3 redox chemical looping. In: Chemical Engineering Journal 421, S. 127734.
[2] Cameli, Fabio; Kourou, Afroditi; Rosa, Victor; Delikonstantis, Evangelos; Galvita, Vladimir; van Geem, Kevin M.; Stefanidis, Georgios D. (2024): Conceptual process design and technoeconomic analysis of an e-ammonia plant: Green H2 and cryogenic air separation coupled with Haber-Bosch process. In: International Journal of Hydrogen Energy 49, S. 1416–1425. DOI: 10.1016/j.ijhydene.2023.10.020
[3] Tong, Lige; Zhang, Aijing; Li, Yongliang; Yao, Li; Wang, Li; Li, Huazhi et al. (2015): Exergy and energy analysis of a load regulation method of CVO of air separation unit. In: Applied Thermal Engineering 80, S. 413–423. DOI: 10.1016/j.applthermaleng.2015.01.074

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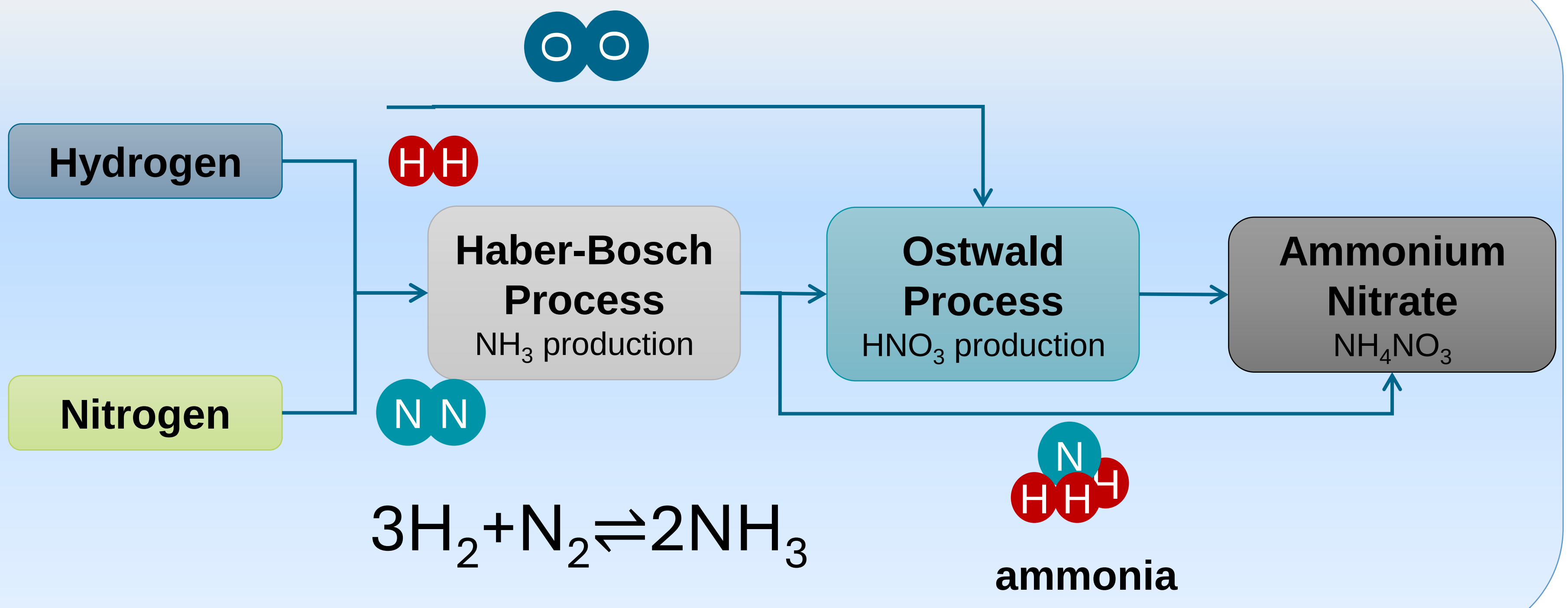
High purity nitrogen production by air separation



$$3H_2 + N_2 \rightleftharpoons 2NH_3$$

Adapted from: Lena Friederike Klaas (2024): Tailoring of Material Properties in Perovskites for Solar Thermochemical Applications. Anpassung der Materialeigenschaften von Perowskiten für solarthermochemische Anwendung

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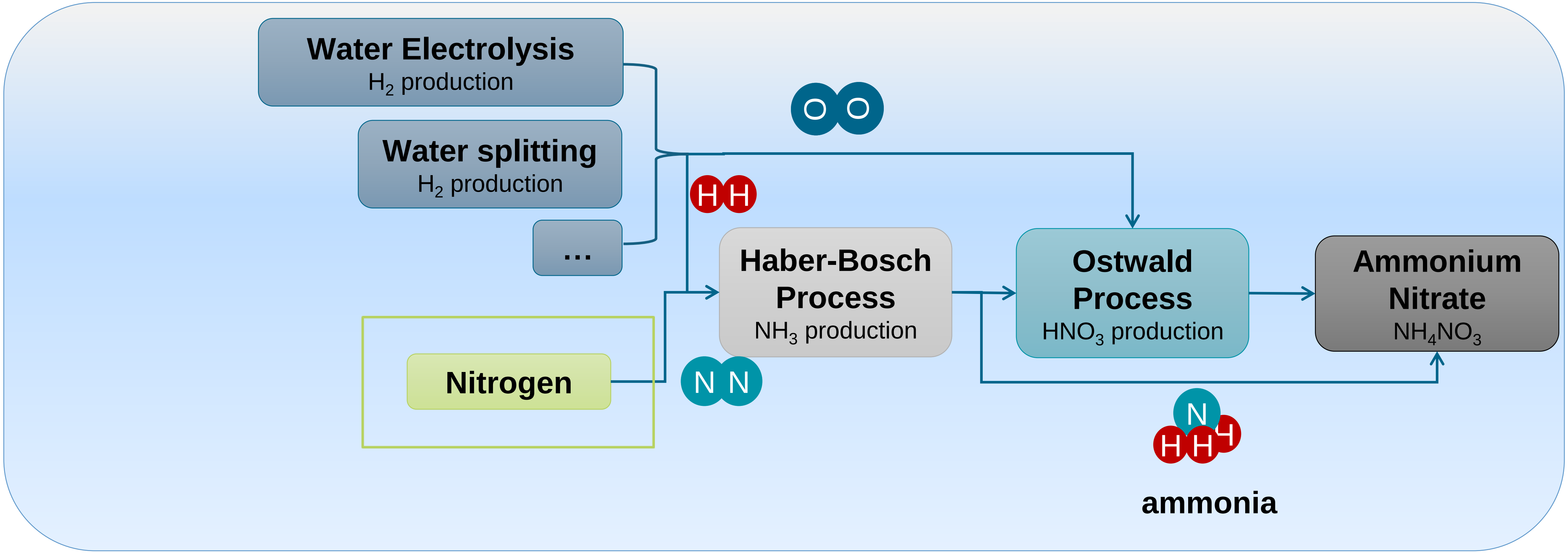

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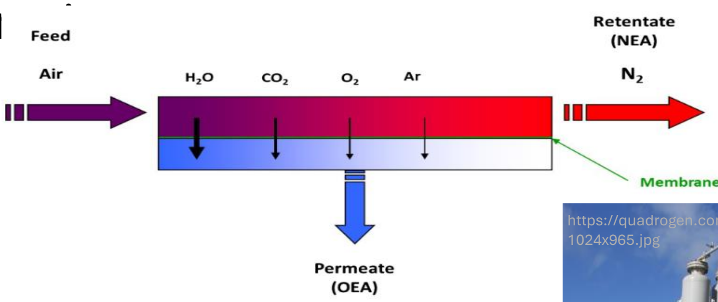
Production of Nitrogen

- ~~Cryog[illegible]paration~~
  - [illegible] energetica[illegible] reasonable on a big industrial scale [3]
  - 2% of the CO_2 emissions of USA and China [1, 2] -> no gree
- ~~Memb[illegible]nology~~
  - only small production capacity [4, 5]
  - maximal purity of 99.9% achievable [4]
- Pressure swing adsorption (PSA)
  - Volume flow ↓↓ & energy consumption ↑↑ for high purity nitrogen
  - Economically only reasonable in combination with thermo-chemical process

combination with thermo-chemical process



[4]

[1] Cameli, Fabio; Kourou, Afroditi; Rosa, Victor; Delikonstantis, Evangelos; Galvita, Vladimir; van Geem, Kevin M.; Stefanidis, Georgios D. (2024): Conceptual process design and technoeconomic analysis of an e-ammonia plant: Green H2 and cryogenic air separation coupled with Haber-Bosch process. In: International Journal of Hydrogen Energy 49, S. 1416–1425. DOI: 10.1016/j.ijhydene.2023.10.020
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[3] Capstick, S.; Bulfin, B.; Naik, J. M.; Gigantino, M.; Steinfeld, A. (2023): Oxygen separation via chemical looping of the perovskite oxide Sr0.8Ca0.2FeO3 in packed bed reactors for the production of nitrogen from air. In: Chemical Engineering Journal 452, S. 139289. DOI: 10.1016/j.cej.2022.139289
[4] Bozorg, M.; Addis, B.; Piccialli, V.; Ramírez-Santos, Álvaro A.; Castel, C.; Pinnau, I.; Favre, E. (2019): Polymeric membrane materials for nitrogen production from air: A process synthesis study. In: Chemical Engineering Science 207, S. 1196–1213. DOI: 10.1016/j.ces.2019.07.029.
[5] Schulte-Schulze-Berndt, A.; Krabiell, K. (1993): Nitrogen generation by pressure swing adsorption based on carbon molecular sieves. In: Gas Separation & Purification 7 (4), S. 253–257. DOI: 10.1016/0950-4214(93)80026-S

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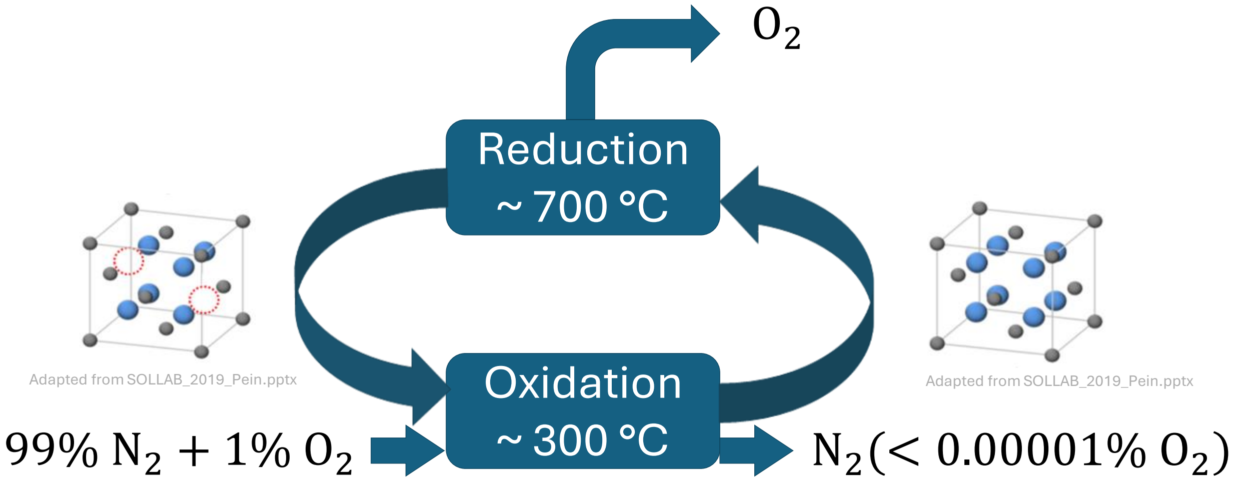
Thermo-chemical air separation

- Perovskites of type ABO_3 absorb & release oxygen
  - Non-stoichometrically
  - Number of oxygen vacancies δ is a function of temperature & pressure [1]
  - No phase-change [1,2]
  - „mild“ reaction conditions [3]

$$ABO_3 \overset{\delta(T, p_{O_2})}{\Longleftrightarrow} ABO_{3-\delta} + \frac{\delta}{2} O_2$$



[1] Bulfin, B.; Vieten, J.; Agrafiotis, C.; Roeb, M.; Sattler, C. (2017), J. Mater. Chem. A 5 (36), S. 18951–18966
[2] Lu, Youjun; Zhu, Liya; Agrafiotis, Christos; Vieten, Josua; Roeb, Martin; Sattler, Christian (2019), Progress in Energy and Combustion Science 75, S. 100785. DOI: 10.1016/j.pecs.2019.100785
[3] Klaas, Lena; Guban, Dorottya; Roeb, Martin; Sattler, Christian (2021), International Journal of Hydrogen Energy 46 (49), S. 25121–25136. DOI: 10.1016/j.ijhydene.2021.05.063.

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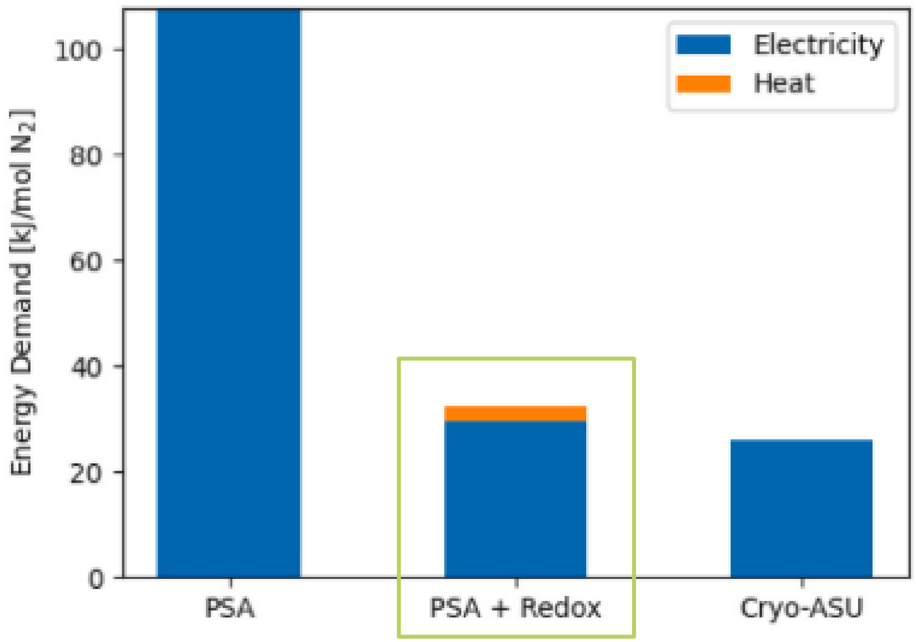
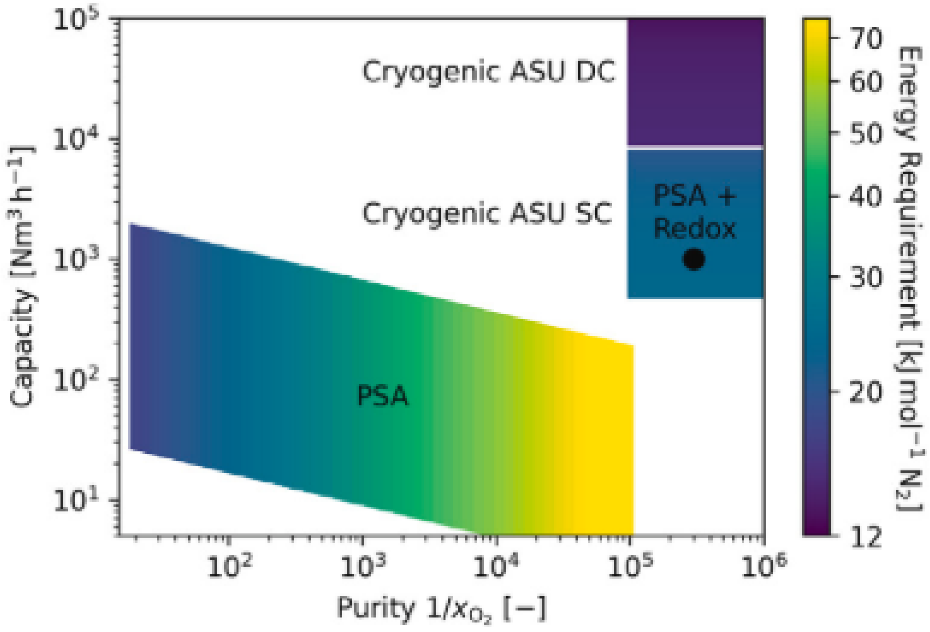
Thermo-chemical air separation & PSA





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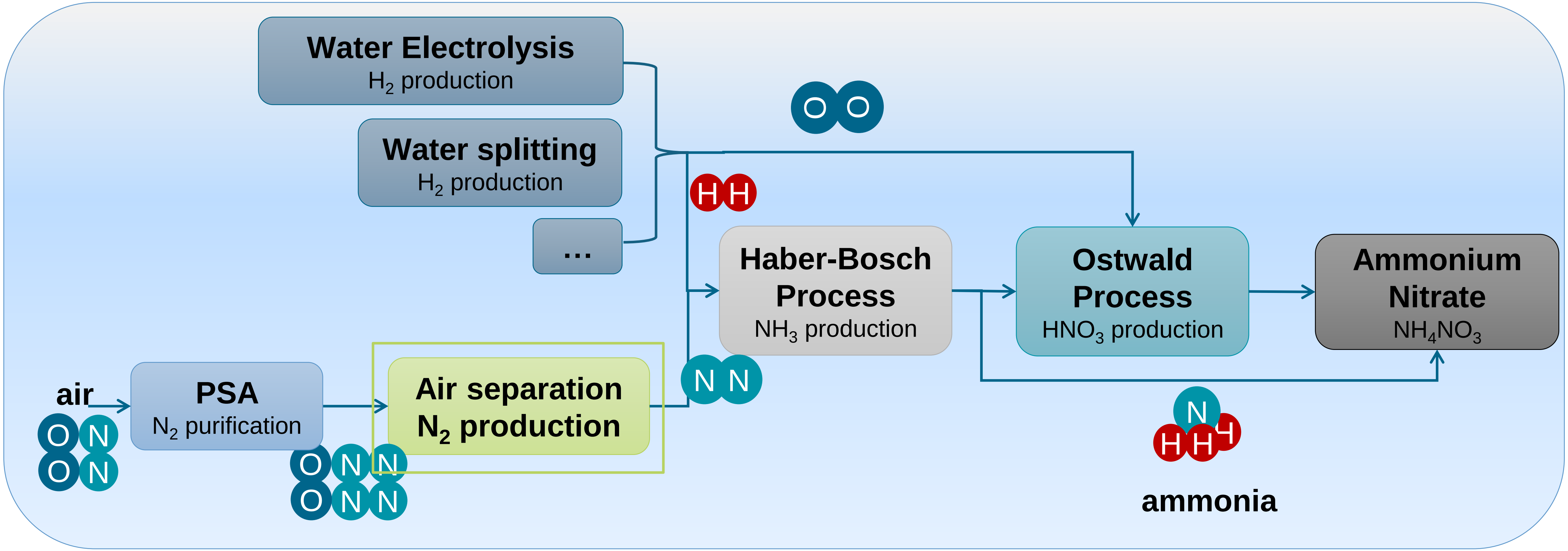
High purity nitrogen production by air separation



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Plans for PhD

- Design of reactor for sustainable production of high-purity nitrogen using
  - Perovskite: $SrFeO_3$ (frequently discussed candidate in literature [1-4])
  - Fixed bed
- Improvement of previous project
- external partners: Exomatter & FGK

Material selection ✓

Process demonstration ✓

PhD:

- Industrial scalability
- Solar integration
- Heat recovery & thermo management

[1] Bulfin, B.; Buttsworth, L.; Lidor, A.; Steinfeld, A. (2021), *Chemical Engineering Journal* 421, S. 127734
[2] Bulfin, B.; Lapp, J.; Richter, S.; Gubàn, D.; Vieten, J.; Brendelberger, S. et al. (2019), *Chemical Engineering Science* 203, S. 68–75
[3] Bulfin, B.; Vieten, J.; Richter, S.; Naik, J. M.; Patzke, G. R.; Roeb, M. et al. (2020), *Phys. Chem. Chem. Phys.* 22 (4), S. 2466–2474. DOI: 10.1039/c9cp05771d
[4] Klaas, Lena; Bulfin, Brendan; Kriechbaumer, Dorottya; Neumann, Nicole; Roeb, Martin; Sattler, Christian (2023), *React. Chem. Eng.* 8 (8), S. 1843–1854
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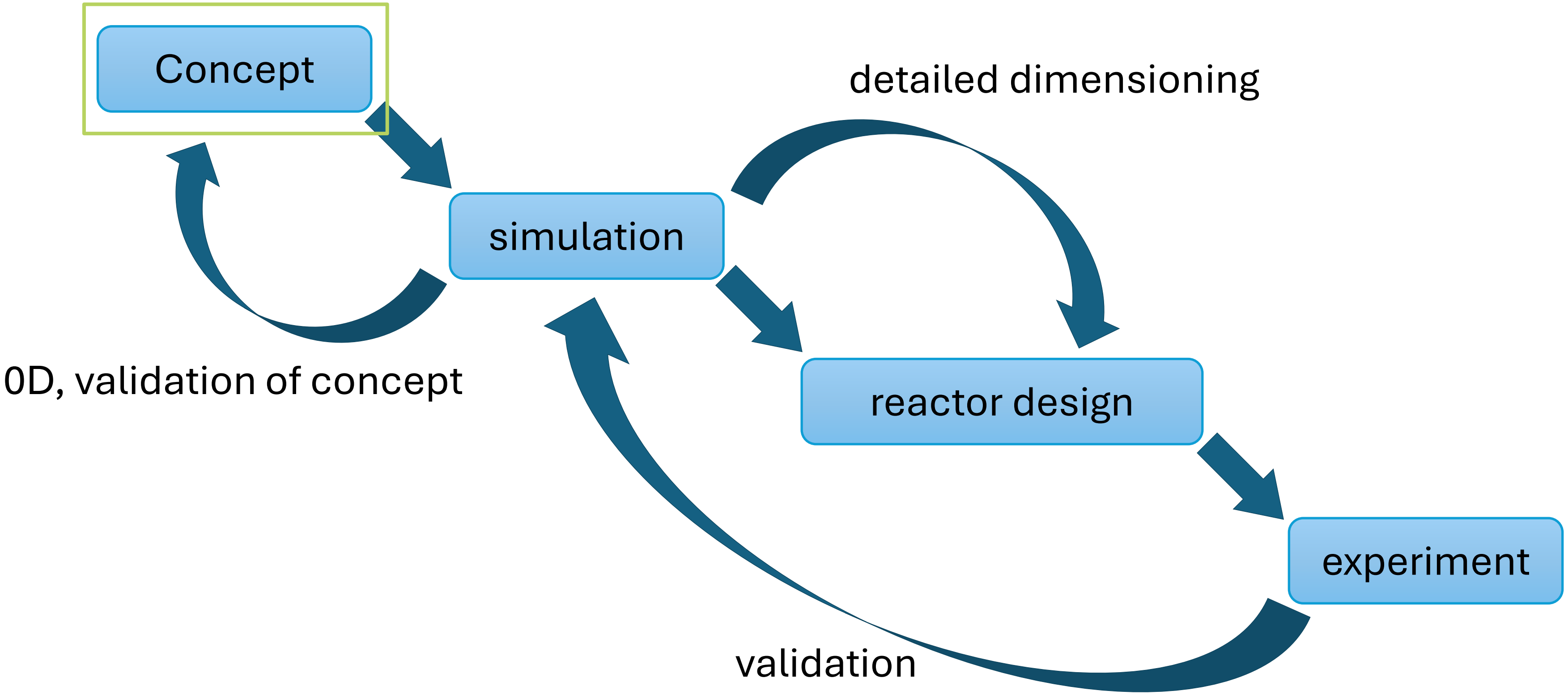
Methodology



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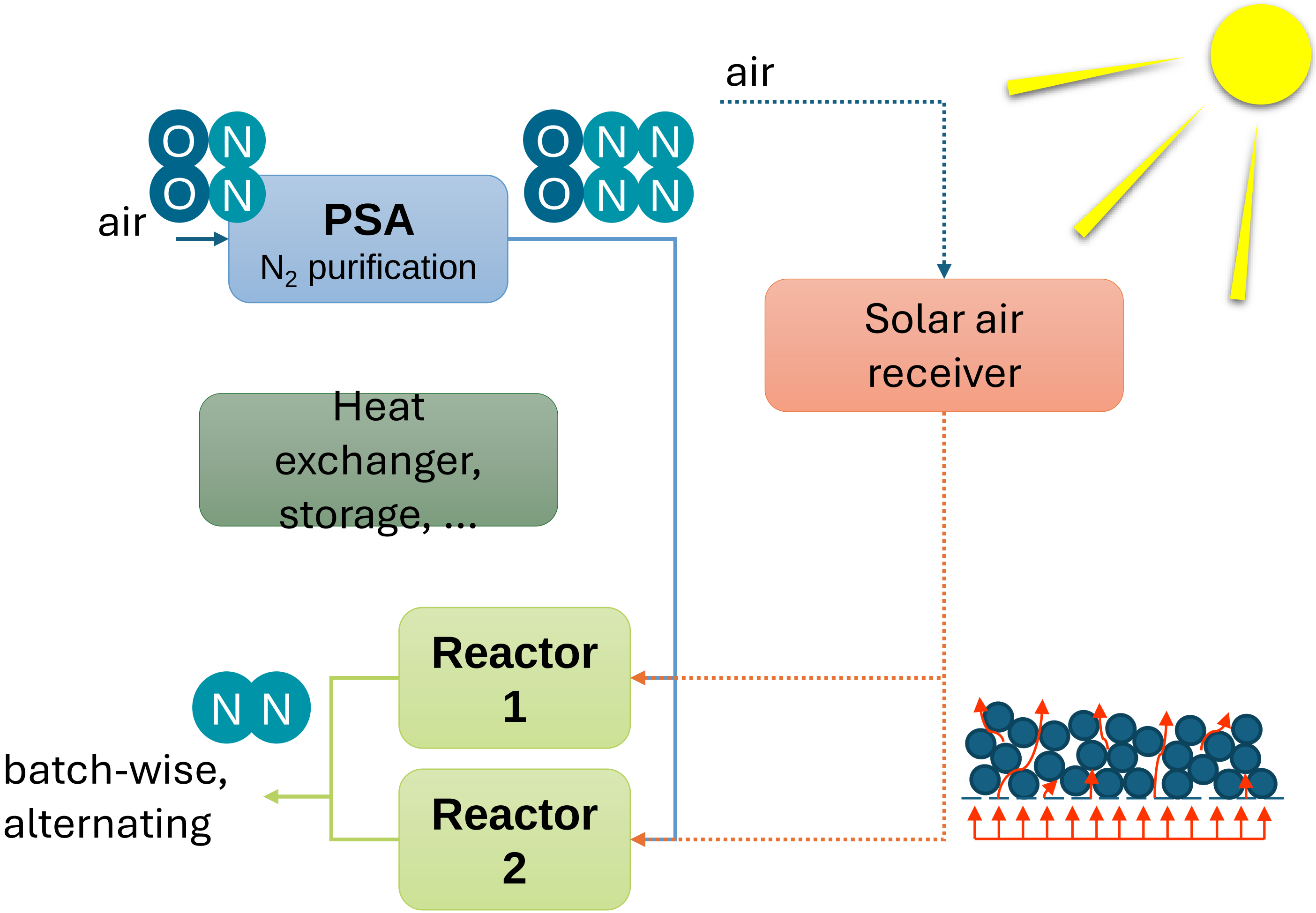

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Concept & Challenges

- Direct heat transfer between gas and fixed bed
  - Heating: warm air from solar receiver
  - Cooling: nitrogen (with max. $1\%\ O_2$) to avoid to early re-oxidation, recircled in a loop
- Possible difficulties
  - Long heating/ cooling durations due to thermal mass
    - Reactor itself needs to be heated/ cooled by independently?!
  - Oxidation & reduction start during heating/ cooling step
    - Negative impact on possible oxygen uptake
- Currently: concept simulation in python (0D)

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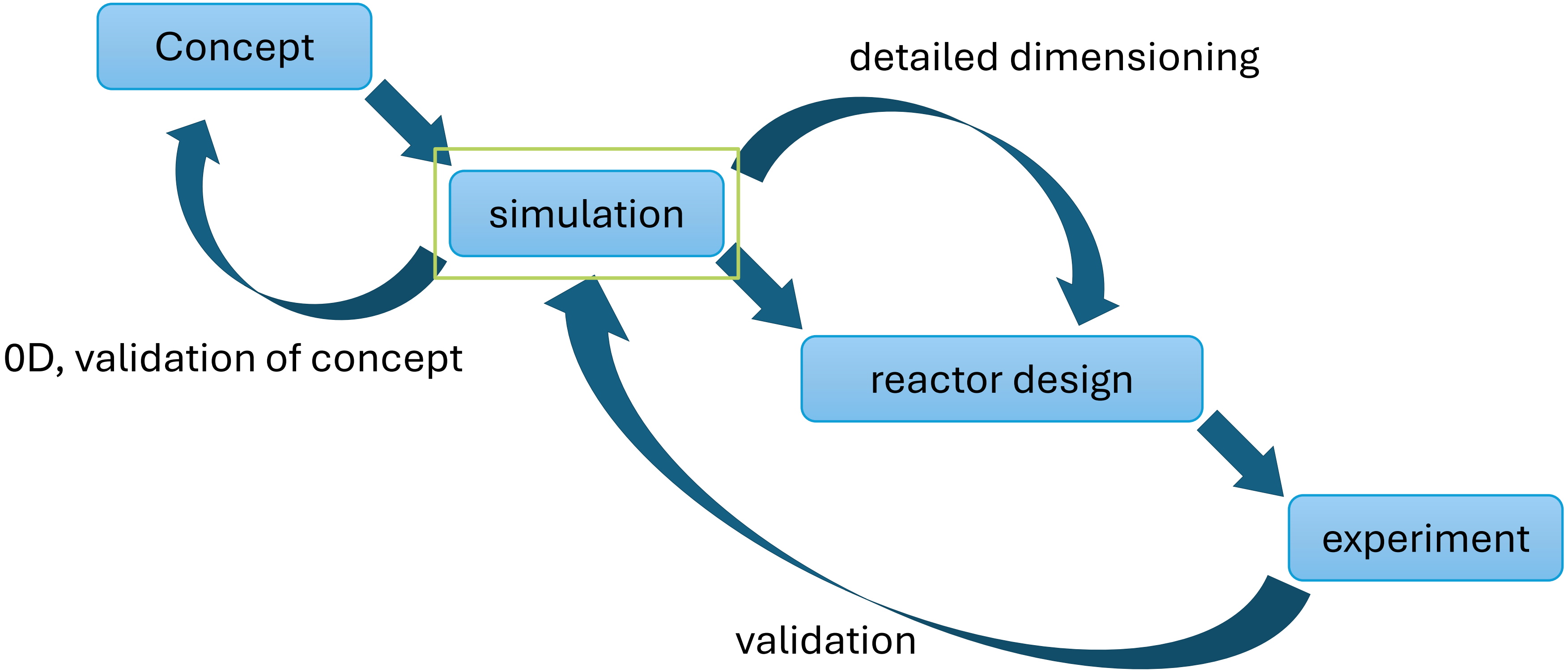

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First simulation results

Simplifications/ current assumptions

- heating/ cooling modelled
- Time-resolved
- No reaction
- 0D
- $\dot{m} = \dot{m}(\eta v_{\mathrm{fluidisation}})$
- Plug flow
- $\lambda_G, \rho_G, c_{p,G}, \mu_G$ = f(T)
- No pressure loss
- Sphericity = 1
- 1 kg of $SrFeO_3$
- $\lambda_P, \rho_P, c_{p,P}$ = const
- Porosity = 0.4 = constant

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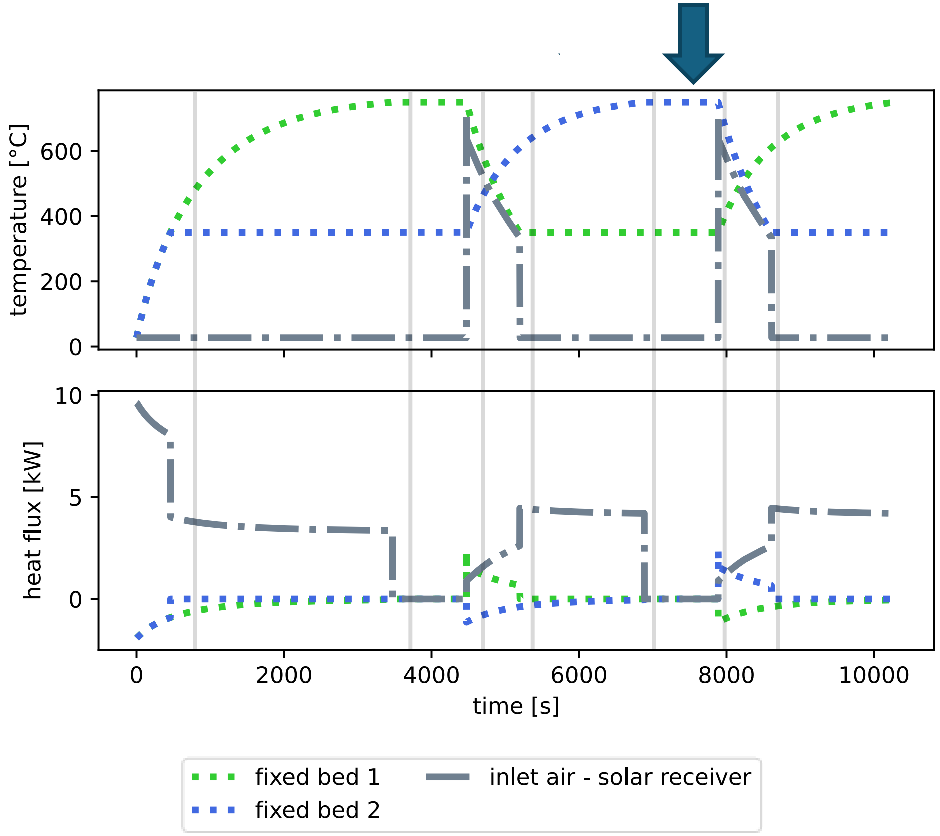

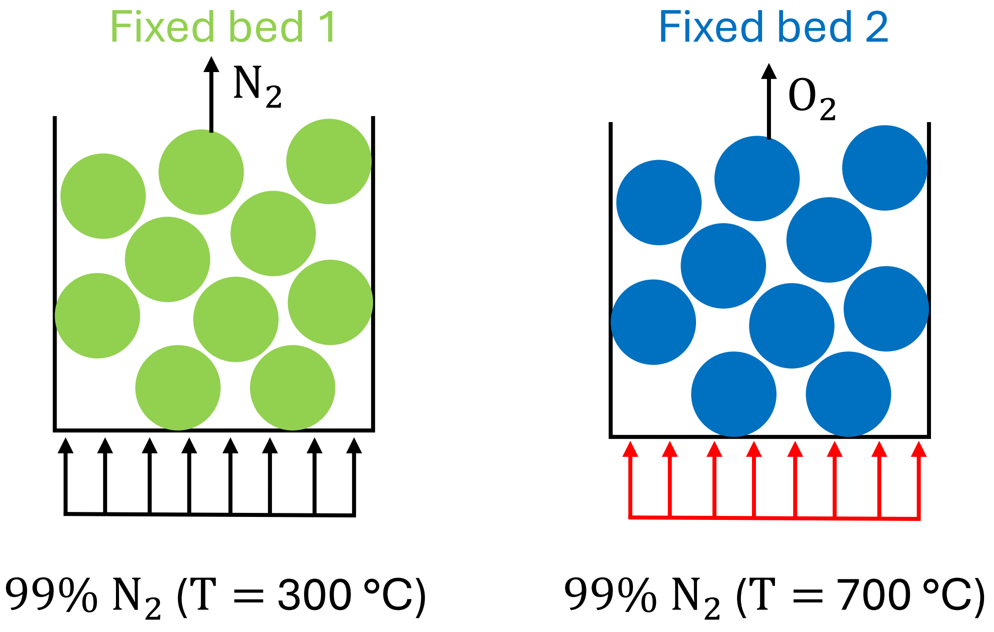

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Outlook & Summary

1st year	Development of reactor concept & Simulation of the concept
2nd year	Detailed reactor design & Preparation of experiments
3rd year	Experimental validation of simulation results

- Fossil-free production of high-purity nitrogen for ammonia production desired
- Development of a reactor for thermo-chemical air separation with redox material $SrFeO_3$
- Concept:
    - Direct heating/ cooling of fixed bed
    - Validation by simulation & experiment

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Imprint

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Date	02.06.2025
Author	Katrin Klingel
Institute	Institute of Future Fuels
Credits	DLR, Lena Klaas, Nicole Neumann, Mathias Pein, Christian Sattler
Disclaimer	Projektträger Jülich, funded by NRW

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