STRATEGIES FOR A MORE RESILIENT GREEN HABER-BOSCH PROCESS

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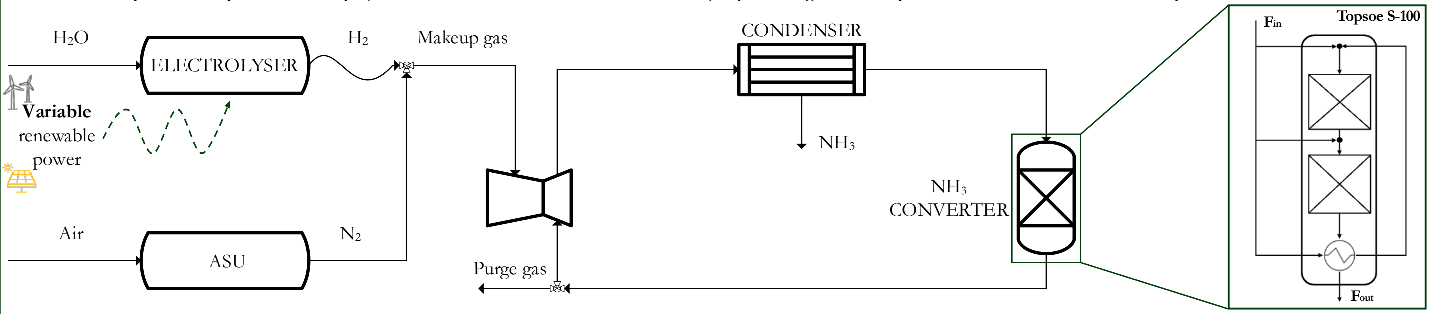
1. Introduction

- In 2020, worldwide production of NH_3 reached around **183 million MT**. Over 96 % of all NH_3 produced comes from the Haber-Bosch (HB) process, which accounts for *c.* **1 – 2 % of global CO_2 emissions** [1].
- Changing the fossil-based feedstock to a greener alternative will help decarbonize the HB process. However, **renewable power fluctuates over time**, meaning H_2 production is not constant. How can the HB synthesis loop be operated if it has traditionally been run at steady-state?

2. Background & research questions

How can the HB synthesis loop be **operated dynamically**?

- Dynamic operation of NH_3 converters is associated with reaction extinction and sustained temperature oscillations [2]. Therefore:
  - **What type of reactor configuration performs best in a Power-to-Ammonia system?**
- Flexibility of the synthesis loop (with and without control measures) operating under dynamic conditions must be quantified.



3. Methodology

- Model **Topsoe S-100 adiabatic quench cooled converter** configuration.

INPUTS — Disturb process variables at the converter inlet:
- Feed flow rate
- Feed temperature
- Mass composition

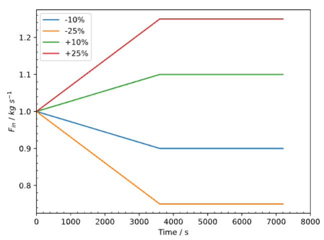
OUTPUTS — Monitor high-level variables:
- Overall conversion
- Axial average fluid/catalyst temperature
- Average residence time per bed

- Goal: develop a disturbance map for a given reactor configuration.

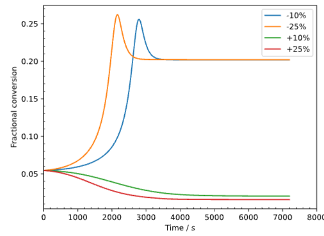
4. gPROMS® FBCR model assumptions

- **System of PDAE** equations defined for the fluid and solid phases.
- **2D model** (axial, z, and radial, r, directions). **Main flow direction is radial**, and axial mixing is considered.
- **Model is heterogeneous**. Catalyst **pellets** are **uniformly reactive** and **lumped**. **Temkin-Pyzhev kinetics** considered, using Dyson-Simon data [3].
- Reactor beds are **adiabatic**.

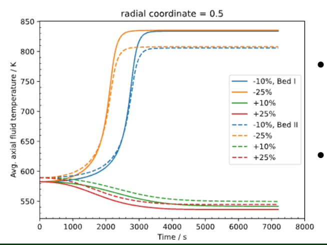
5. Results



Disturbance in the converter feed flow rate, F_{in}:
- Type: **Ramp**
- Duration: 3600 s
- Magnitude: ± 10 % & ± 25 %



- **Increased conversion** when $\mathbf{F_{in}}$ **is reduced**, due to greater solid-fluid contact time.



- Fluid temperature captured when r = 0.5 and averaged along the z-direction.
- **Fluid temperature increases** when $\mathbf{F_{in}}$ **decreases**. Higher conversion higher fluid temperature.

6. Conclusions and Future Work

- This analysis, which clarifies the intricate mass and energy dynamics of these converters, will be applied to other reactor configurations.
- Through a comprehensive set of dynamic tests, the best reactor configuration for Power-to-Ammonia applications can be determined and subsequently tested within the synthesis loop.

References:

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