PhD Open Days

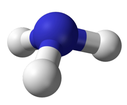
Flexibility Analysis of a Haber-Bosch Loop for Power-to-Ammonia Systems

Ph.D. Program in Chemical Engineering

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Introduction

- Ammonia (NH_3) is produced via the Haber-Bosch (HB) process that accounts for *c*. **1-2 % of global CO_2 emissions** [1].



- Transitioning from fossil-based to renewable feedstocks leads to **fluctuating green-feedstock production**, while the HB synthesis loop has been traditionally **operated near steady-state** [1].

Objectives

- **Quantify** the ***dynamic flexibility*** **of a synthesis loop design without control measures**, building on previous dynamic modelling work [2].
- **Develop** a preliminary **operational map** for the loop flexible-load operation.

Methodology

- Development of a gPROMS® Process **flowsheet model** for a **4 kt NH_3/year synthesis loop** with a **quench-cooled converter**, reproducing Topsoe's S-100 converter.
- **Dynamic tests on the fresh make-up flow rate** to reproduce operation scenarios, thereby enabling:
  - (i) The **identification** of **operational constraints;**
  - (ii) The **construction** of a preliminary **operational map**.

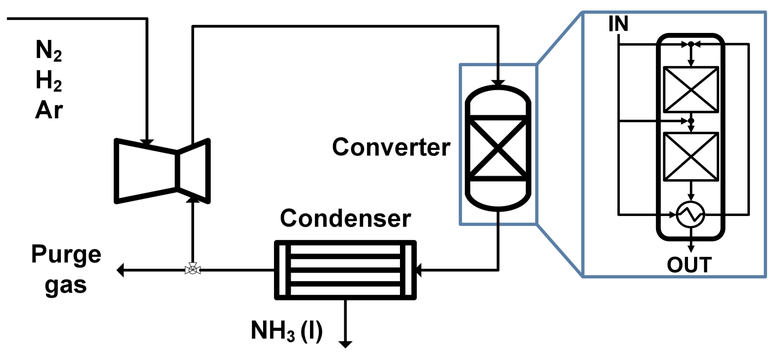


FIGURE 1: Process flow diagram of a NH_3 synthesis loop.

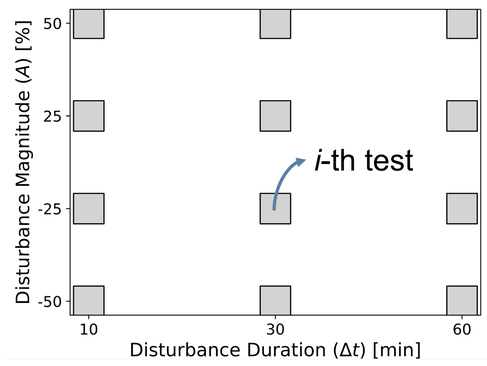


FIGURE 2: Test matrix considered in this work.

Results

- For all tests conducted, **only catalyst bed overheating and reaction extinction** were observed.

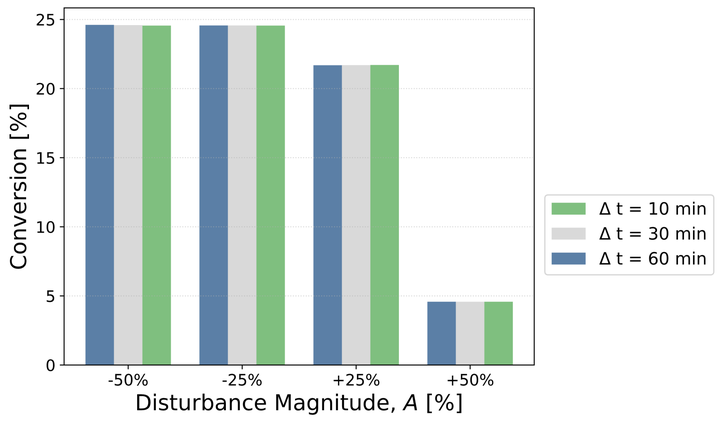


FIGURE 3: Per-pass conversion (after the dynamic test) as a function of disturbance magnitude and duration.

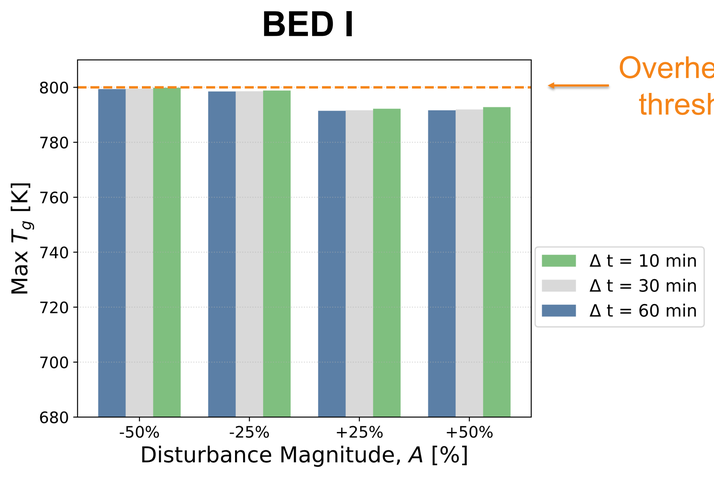


FIGURE 4: Maximum recorded bed I temperature as a function of disturbance magnitude and duration.

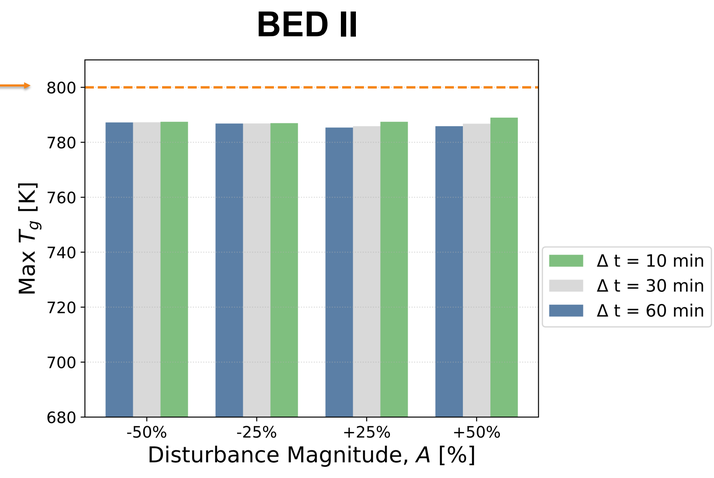


FIGURE 5: Maximum recorded bed II temperature as a function of disturbance magnitude and duration.

- Reaction **virtually extinguished** for all + 50% disturbances.
- Disturbance time has no influence on the system's observed behaviour.
- For bed I, slight catalyst bed overheating is observed due to lower molar flow rate entering the converter.
- **Disturbance magnitude serves as a metric for system flexibility.**

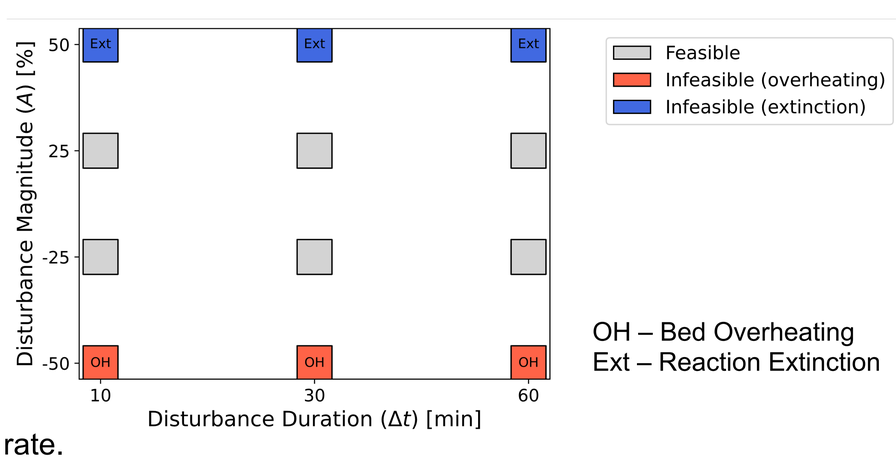


FIGURE 6: Operational map for loop disturbances on the make-up flow rate.

Final Remarks

- Results indicate that the loop is, at least, flexible by ± 25% in its current configuration, with no influence of the disturbance time on the results.
- Implement design-based flexibility measures in the flowsheet and assess the resulting flexibility.

References:
[1] Narciso, D. A. C. *et al.* (2025). Design and operation of Power-to-Ammonia Systems: A Review. *Ener. Conv. Manag.*, 327, 119494
[2] Pires, J. M. *et al.* (2025). Strategies for a More Resilient Green Haber-Bosch Process. In *Book of Short Papers 35th European Symposium on Computer Aided Process Engineering*, EUROSIS-ETI.

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