ARENHA Webinar

Process simulation for absorption-assisted ammonia synthesis

5th December 2023

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862482

Gerard van Zee

Gerard.van.Zee@protonventures.com

About Proton Ventures

EMPOWERING AMMONIA SOLUTIONS

Chemicals, green energy and beyond

Since its foundation in 2001 Proton Ventures has been a pioneer in the (green) ammonia industry:

- 22 years pioneers and developers in (green) ammonia
- Technology agnostic engineering & system integrator
- Entire green ammonia value chain knowhow
- International team of specialists
- In house engineering disciplines & certifications

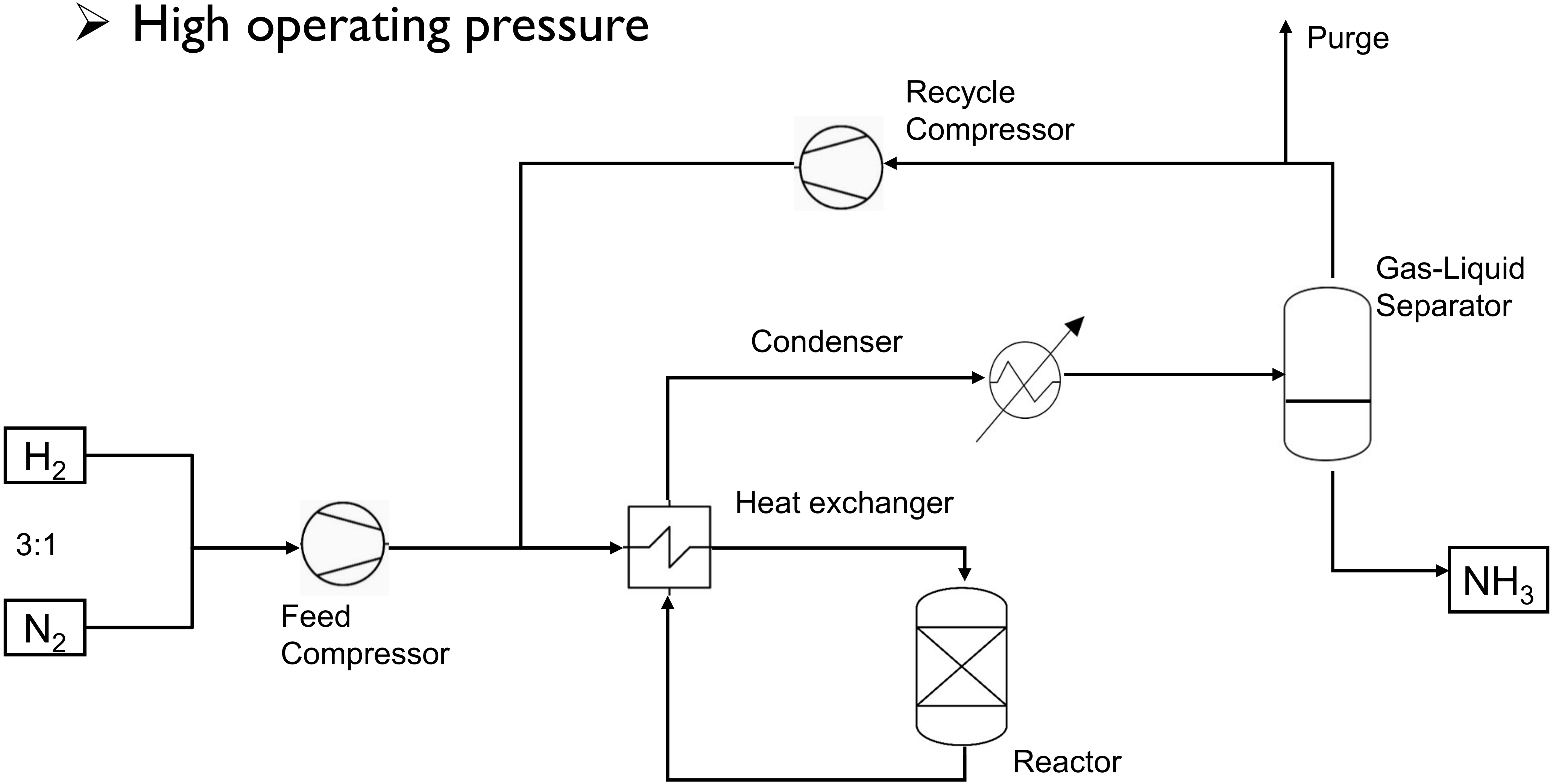
From concept to operational facilities, Proton Ventures offers consultancy support, project development management, feasibility study and FEED study engineering services, up to and including the actual EPC works.

ARENHA tasks

Design and construction of the ARENHA pilot plant for ammonia synthesis

Typical Haber-Bosch ammonia plant schematic

- $3\ H_2 + N_2 \leftrightarrow 2\ NH_3$
- Strongly exothermal reaction
- High operating pressure

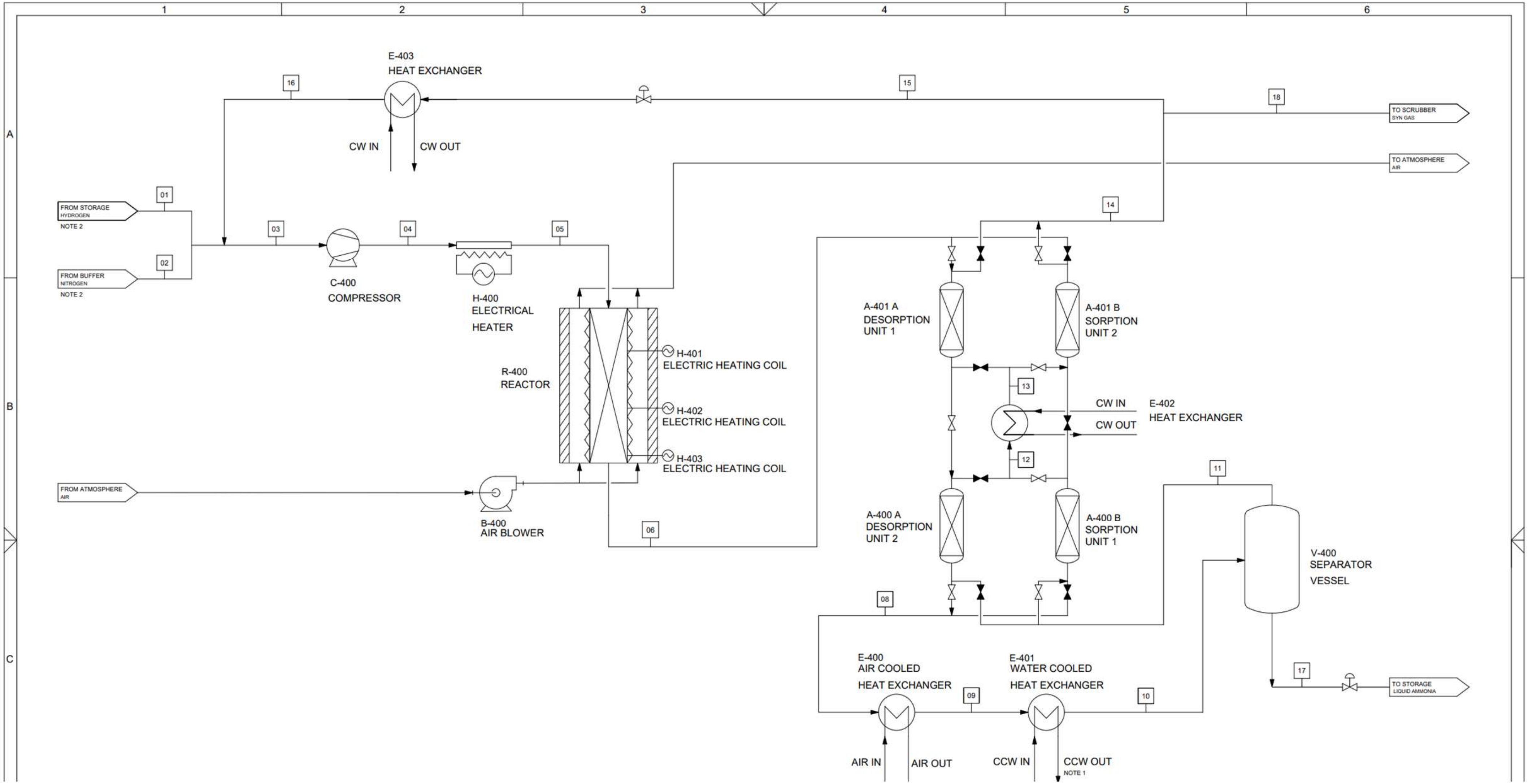


Webinar
05-12-2023

ARENHA objectives and conditions

- Ammonia pilot unit of scale size 10 kg/day ammonia
- Enhanced ammonia recovery using absorption by novel metal halide sorbents
- Suitable for operation at variable capacity
- Liquid product storage at ambient temperature

ARENHA synthesis Process Flow Diagram



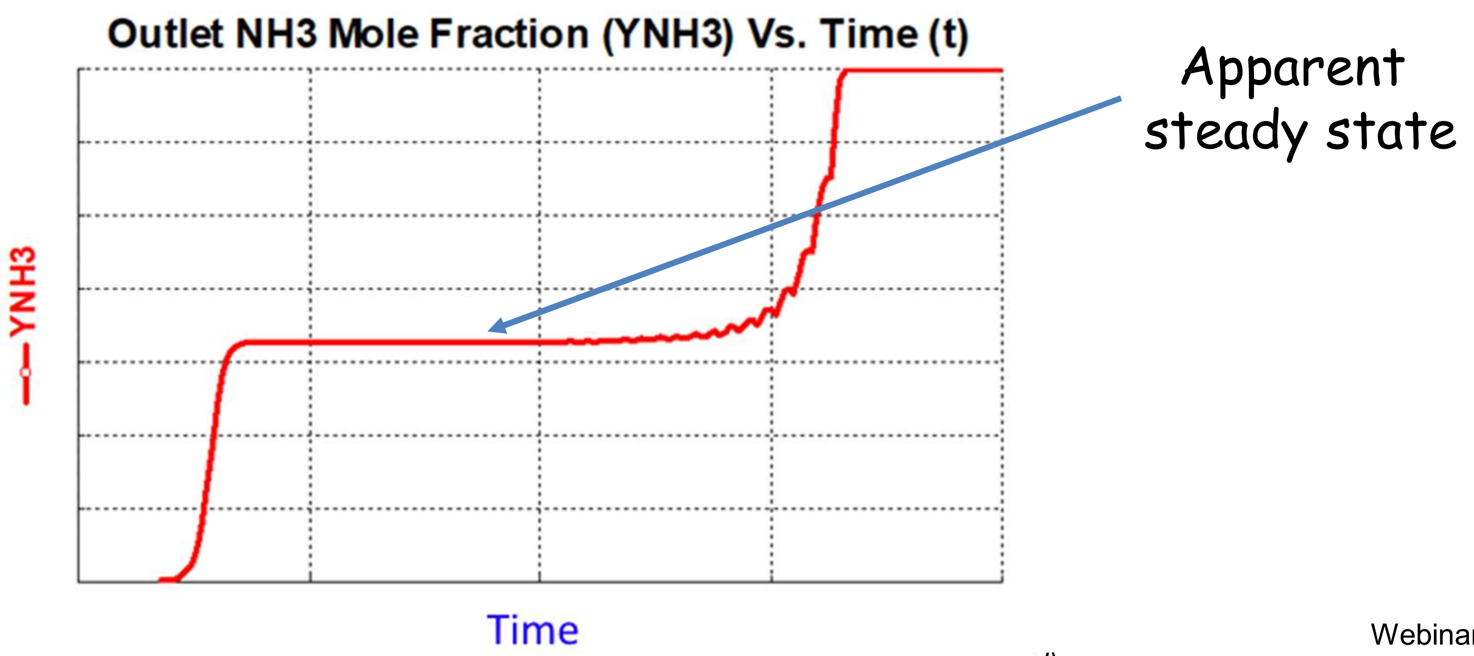
Webinar
05-12-2023

ARENHA plant simulation

- Constructed in the Aspen Plus environment
- Required for equipment sizing and specification
- PFR reactor model with kinetics model for selected catalyst
- Steady state
- Absorption incorporation as quasi-steady state operation

Absorber properties examination

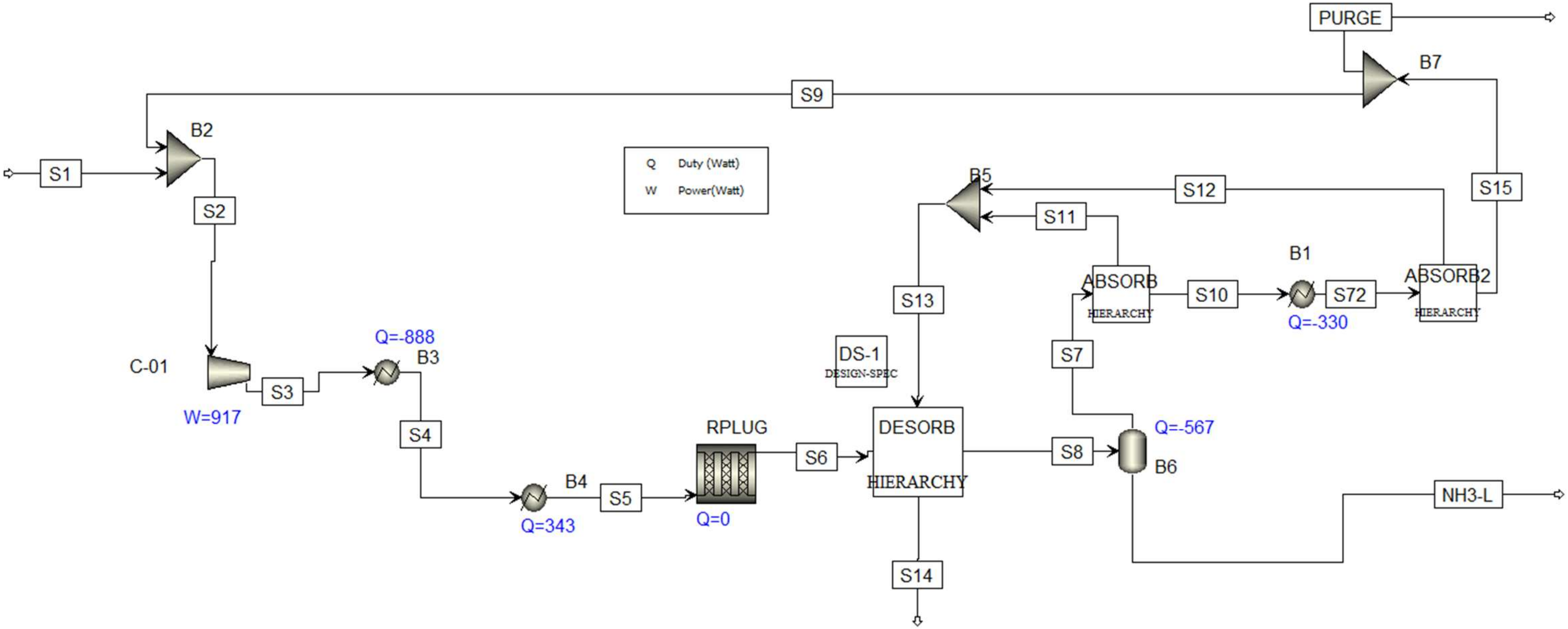
- Advanced metal halide sorbent material developed by DTU
  - Active layer on pore surface of granular carrier material
- sorption behavior analysis using ***Aspen Adsorption*** *model*, based on:
  - Adiabatic sorption column
  - $P_{sat}(T)$ for $MgCl_2$-based absorbent
  - Adsorption isotherm is independent of concentration NH_3 in sorbent
  - Estimated pore diffusion resistance



d).

Aspen model for Arenha synthesis process

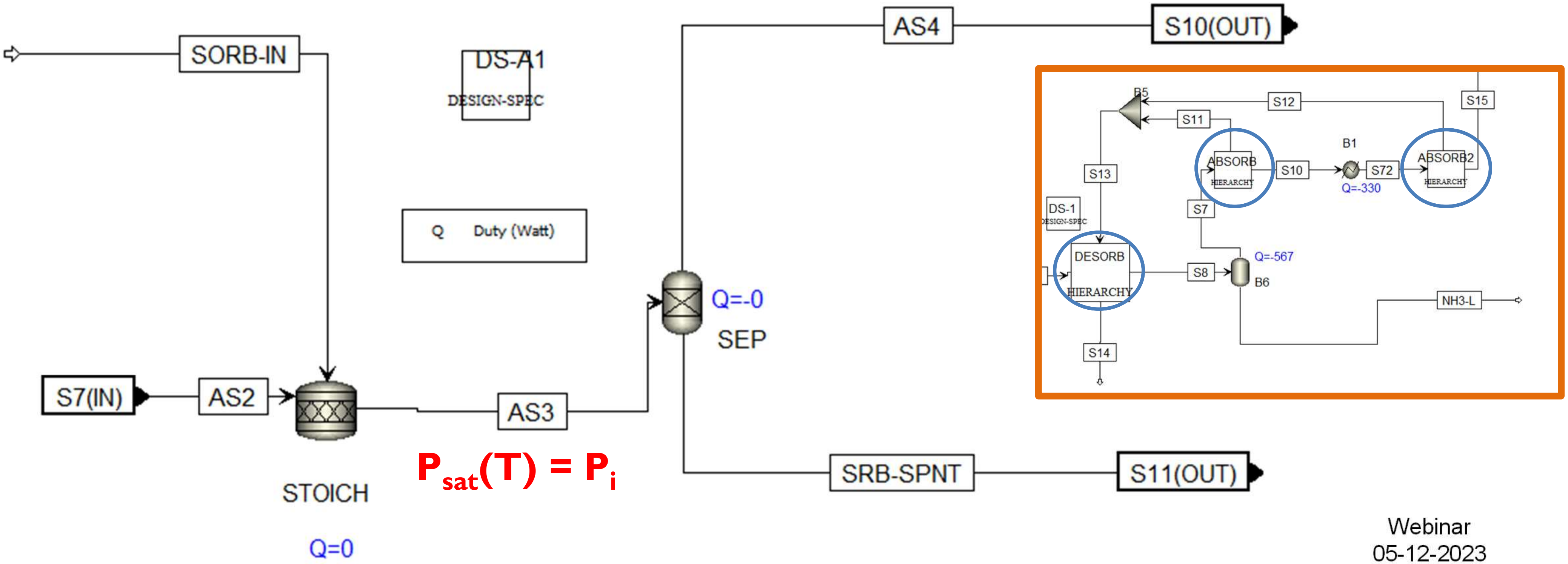
- Constructed in the Aspen Plus environment
- Solid phase stream introduced for quasi steady state absorption



Process model: Sorption UO

- Solid phase has the thermodynamic props (ΔH, c_p) of actual sorbent.
- Sorption equilibrium is reached at:

  Saturated vapor pressure P_{sat} for sorbent = partial vapor pressure P_i.
- Aspen Fortran routine controls solid sorbent feed flow rate in order to obtain equilibrium at reactor discharge *AS3*
- For regeneration step: Solid sorbent feed flow rate given, regeneration extent is verified



$P_{sat}(T) = P_i$

Process modelling results

- Functional steady-state process simulation model, to complete the PFD.

- Process configuration is easy to automate, budget compliant and well suitable for experimentation.

- More rigorous modeling required for absorption and regeneration process for column sizing.
  (in COMSOL by Technical University of Denmark)

Dynamic process modelling

- For varying H_2 feed flow rates, as anticipated for green hydrogen

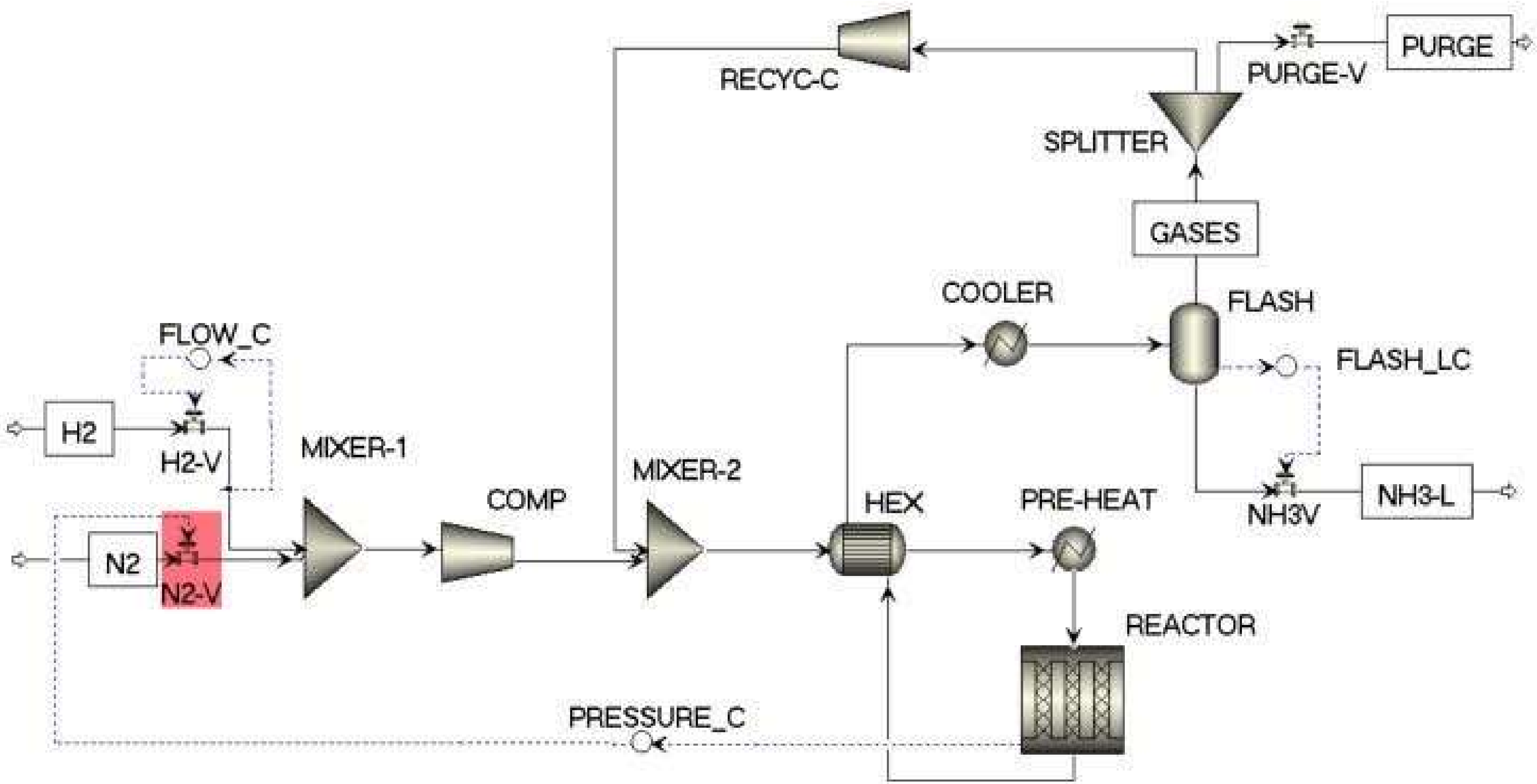
- Cause for strong operating pressure fluctuation.

- Potential cause of equipment damage by metal fatigue

- Three control principles investigated to maintain operating pressure:
  A. Nitrogen excess feed control, acting as inert
  B. Recycle flow rate control
  C. Condenser cooling duty

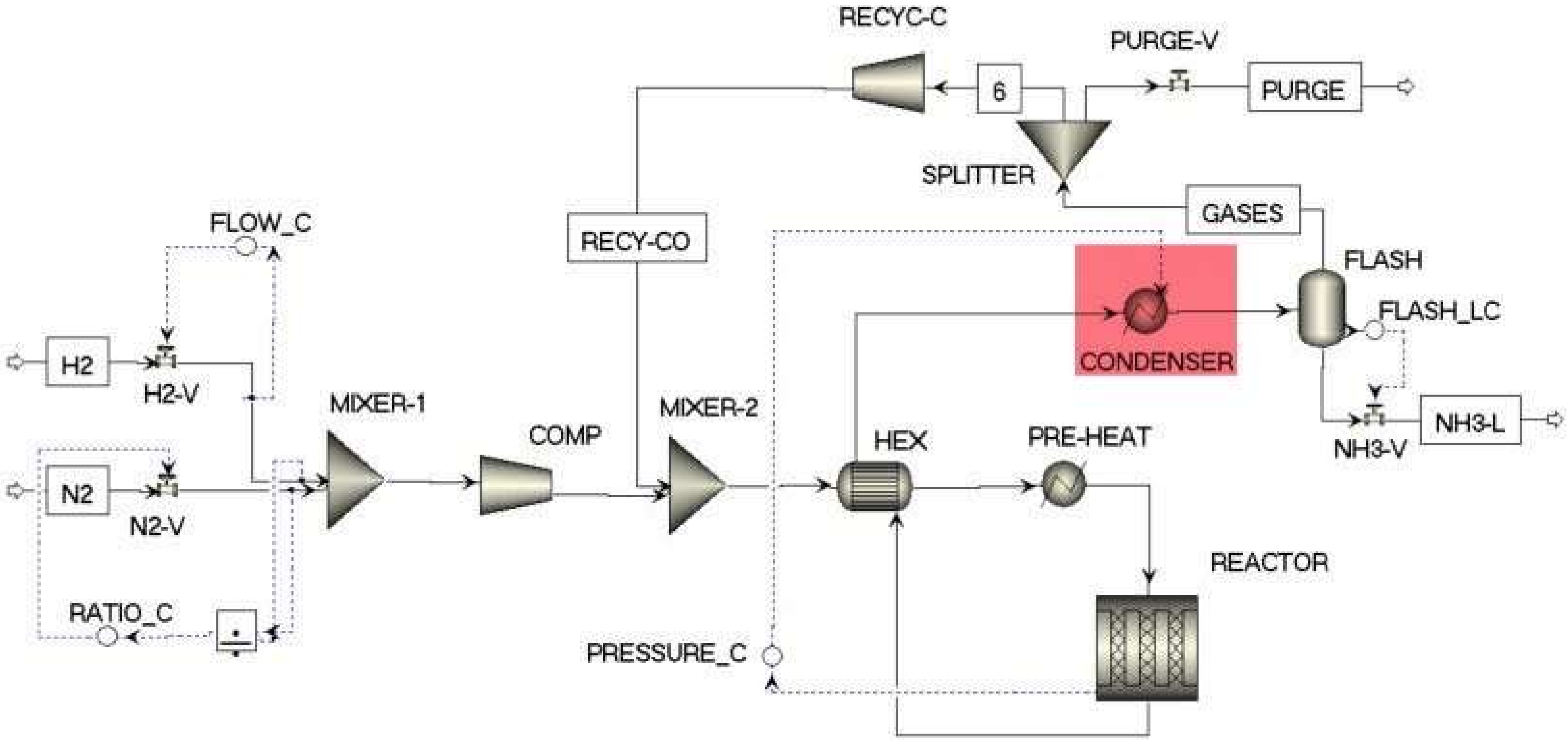
Dynamic process modelling

➢ A. Loop pressure controlled by excess nitrogen feed flow rate

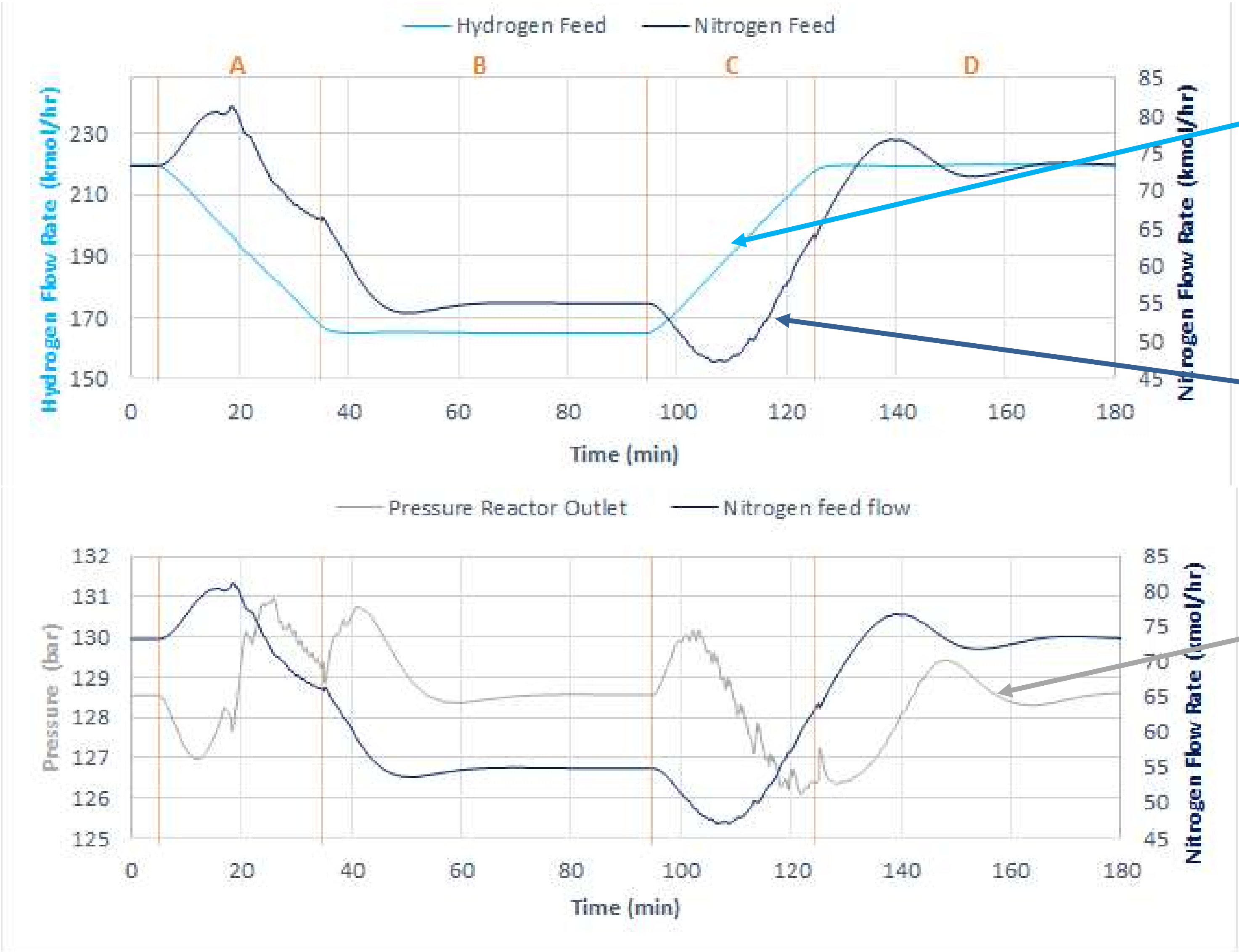


Dynamic process modelling

➢ C. Loop pressure controlled by condenser cooling duty



Dynamic process modelling A result



H_2 feed upset and recovery

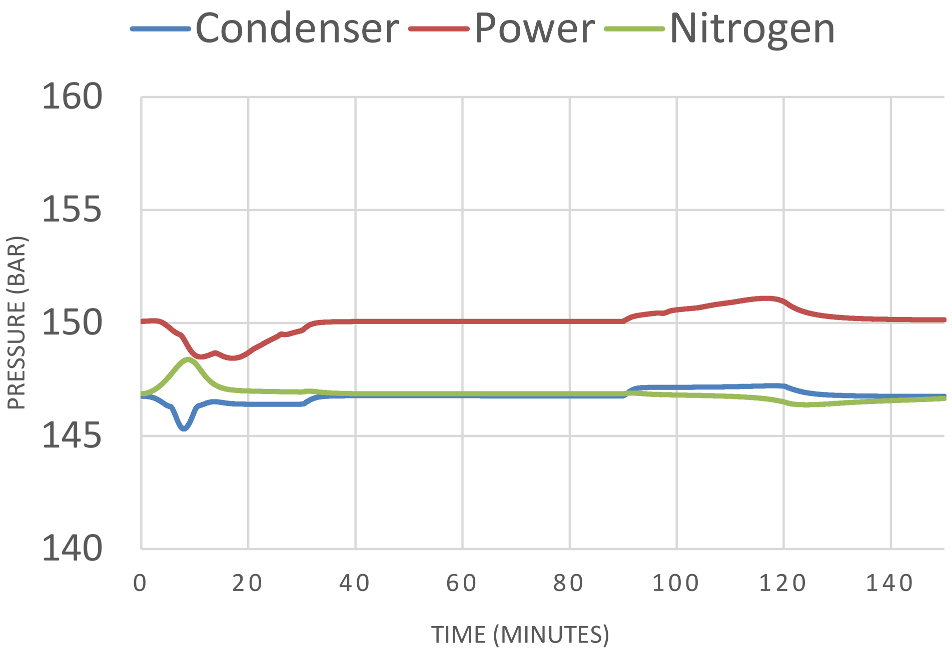
Controlled N_2 feed flow rate response

Pressure fluctuations remain small

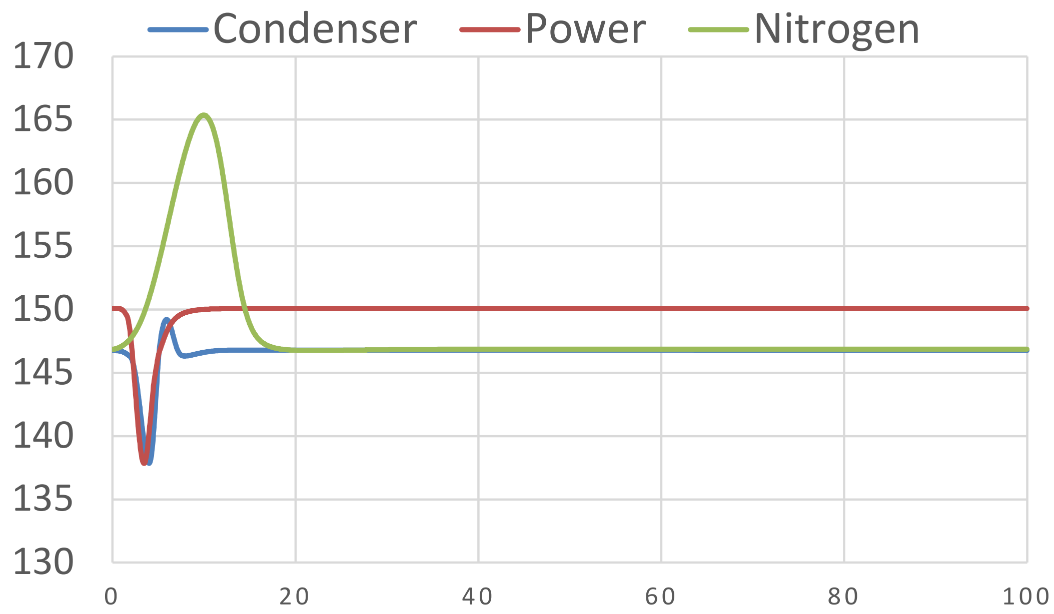
Webinar
05-12-2023

Control strategy comparison

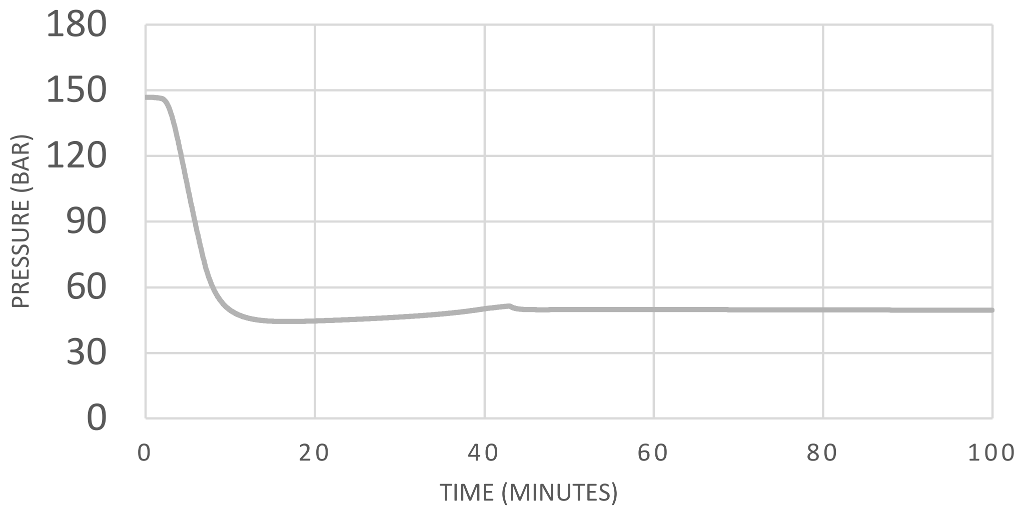
50% LINEAR H_2 REDUCTION



50% STEP H_2 REDUCTION



No pressure control



Dynamic simulation results

- Operation at varying feed flow rates feasible for all three control philosophies tested
  - H2/N2 feed ratio control
  - Recycle flow rate control
  - Condenser cooling duty control

- No limitations observed in ramp-down rate or in H_2 feed flow rate minimum

- H_2 feed flow variation restricted only by feed compressor operation limitations

ARENHA demo plant realization

- Process simulations results used for:
  - Process Flow Diagram (PFD)
  - Process & Instrumentation Diagrams (P&ID)
  - Equipment sizing and compile data sheets

- Manufactured by DEMCON Suster Sustainable Process Solutions

- To be delivered as skid for installation at CNH2\Fertiberia site

Advanced materials and Reactors for Energy storage tHrough Ammonia

areNH3a

Thank you for your attention