MODELLING AND SIMULATION OF SMALL SCALE POWER-TO-AMMONIA WITH APROS VIRTUAL PLANT

Teemu Sihvonen & Jouni Savolainen, VTT

7th Researchers' Seminar, Lappeenranta 24.1.2017
CONTENTS

• Ammonia in general
• Small scale ammonia production
• Methods of study
• Results
Ammonia in general

- NH₃
- One of chemical industry’s ~20 basic products (Gani, 2004)
  - Precursor to e.g. fertilizers
  - Fuel
- Production traditionally in centralized, large scale plants
  - Size > 1000 t/d
  - Haber-Bosch process, Fe catalyst, 400-500°C, ~300bar
  - Transportation costs to remote locations?
  - Energy intensive
    - H₂ by steam reforming of CH₄: 1.2% of global primary energy demand (Gilbert and Thornley, 2010)
    - N₂ from air (cryogenic or PSA)
  - Carbon emissions: 0.93% global GHGs (IFA, 2009)


Small scale ammonia production

- Two less carbon intensive ways
  - Biomass gasification
    - $\text{H}_2$ from gasification, $\text{N}_2$ from air or gasifier
  - Renewable powered
    - $\text{H}_2$ from electrolysis, $\text{N}_2$ from air
- We study the latter
  - Distributed fertilizer source
  - Energy storage
  - Farming equipment fuel
  - High wind power potential & high ammonia demand meet (Reese, 2016)

Figure 2. Ammonia demand in the United States. The regions of greatest ammonia demand, shown as the darker areas, roughly coincide with the areas of greatest potential wind energy. (Figure adapted from ref 15.)
How?

1. Laying the groundwork
   – Kinetics, Froment & Bischoff, 1990
   – Material properties: Look-up tables as functions of T and p for $\lambda$, $\mu$ and $C_p$
   – Programming…

2. Verification of kinetics
How?

3. Process modelling
   • Scope
   • Size: 5 MW<sub>e</sub>
   • Unit operations development
     – Synthesis loop
     – PSA
   • Control logics development
     – Partial start-ups and shutdowns
     – Altering feed to the synthesis

   • Expert validation
How?

4. Operational optimization
   - Robust optimization in similar manner as in PtG case
     - More information available from Robert Weiss

5. Reporting @ IRES’2017
   - Robust Optimization And Dynamic Simulation Of A Small Scale Power-To-Ammonia Plant;
     Weiss, Robert; Savolainen, Jouni; Tähtinen, Matti; Sihvonen, Teemu; Bennani, Yasmina; Hans, Vincent; Vrijenhoef, Hans
Results

• Capabilities development
  – Tools to study & design NH$_3$ process dynamics / control
  – Example simulations
    • Optimal running schedule from optimization
    • See next slides

• WP6 related
  – Joint publication with Proton Ventures
  – Invitation to the 1$^{\text{st}}$ European Conference on Power to Ammonia
    • 18-19.5.2017, Rotterdam
Results

- Total power to PEM units (MW)
- Number of operating PEM units
- Mass flow [kg/s] for H₂ and N₂
- Pressure [MPa] for H₂ and N₂ storage

NEO CARBON ENERGY
Next

- Finalize IRES paper
  - Deadline is 31.1.2017

- Power-to-X
  - Dynamic rWGS and static F-T: Jouni, Paco, Matti R.

- Integration of biomethanation unit operation model to Virtual Plant: Teemu, Eero

- Extension towards fertilizers: Robert, Ilkka H.

- Virtual Plant documentation: all

- ”WP4 Summary Case”: all
  - On the drawing board…