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**Modeling the Carbon Footprint of Ammonia Production via the Haber-Bosch Process**

**Objective**: Estimate the carbon footprint of conventional ammonia production and a greener alternative (e.g., electrochemical synthesis using green hydrogen) and compare them using process modeling and life cycle analysis tools.

**Step 1: The Haber-Bosch Process (How Ammonia Is Synthesized Industrially):**

Equation: N2​(g)+3H2​(g)→2NH3​(g)

Key Inputs: Nitrogen (from air), hydrogen (from natural gas via steam methane reforming).

Outputs: Ammonia + CO2 (from Hydrogen production).

**Energy consumption data and CO2 emission factors for each component:**

**Component 1: Steam Methane Reforming (SMR)**

* Purpose: Produces hydrogen (H2) by reacting methane (CH4) with steam.
* Energy Consumption:
  + 28 – 30 GJ/tonne NH3
  + (Source: IEA 2021, Ullmann’s Encyclopedia of Industrial Chemistry)
* CO2 Emissions:
  + Direct emissions from reaction:
    - CH4 + H2O→CO + 3H2
    - CO + H2O→CO2 + H2
  + Combustion of CH4 for heat:
    - ~56.1 kg CO2 per GJ natural gas used
  + Total CO2 from SMR:
    - Roughly 1.6-1.9 tonnes CO2/tonne NH3
* Emission Factor Source:
  + U.S. EPA, IPCC Guidelines, Ecoinvent database

**Component 2: Air Separation Unit (ASU)**

* Purpose: Extracts nitrogen (N2) from air for ammonia synthesis.
* Energy Consumption:
  + 0.2 – 0.4 GJ/tonne NH3 for cryogenic separation
  + (Source: DOE reports on industrial air separation)
* CO2 Emissions:
  + If powered by grid electricity:
  + 0.4 GJ x 277.78 = 111.1 kWh
  + 111.1 kWh x (0.5 kg CO2)/kWh ≈ 56 kg CO2

**Component 3: Ammonia Synthesis Reactor (Haber-Bosch)**

* Purpose: Reacts H2 and N2 under high pressure and temperature.
* Energy Consumption:
  + 2-3 GJ/tonne NH3 for:
    - Compressors (up to 300 atm)
    - Heaters to reach 400-500°C
    - Source: IEA, ChemEng design texts
* CO2 Emissions:
  + Primarily from electricity or heat sources:
    - 3 GJ = 833.3 kWh ⇒ 833.3 x 0.5 = 417 kg CO2 (approx.)

**Summary Table**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| **Component** | **Energy Use (GJ/tonneNH3)** | **Main Fuel Source** | **CO2 Emission Factor** | **Est. Emissions (kgCO2/tonneNH3)** |
| SMR (H2 production) | 28-30 | Natural gas (CH4) | 56.1 kg CO2/GH | 1,600-1,900 |
| ASU (N2 production) | 0.2-0.4 | Electricity (grid) | 0.5 kg CO2/kWh | ~56 |
| NH3 Reactor (compression & heat) | 2-3 | Electricity/natural gas | 0.5 kg CO2/kWh | ~417 |

* Additional Resources: PubChem, NIST WebBook, “Green Ammonia: Impact of Fertilizer and Fuel”

**Step 2: Modeling the Process Flow**

**Tool:** [DWSIM](https://dwsim.org/)

**How much NH3 was formed:** 8.332044 kg/s

**How much unreacted H2 is left:** 24.876913 kg/s

**How much unreacted N2 is left:** 23.902160 kg/s

**CO2 produced from SMR:** 143.85 kg/s

**DWSIM Flowsheet Is Included in GitHub Profile**

**Step 3: Estimating the Carbon Footprint**

1. **CO2 from SMR:** 143.86 kg/s
2. **CO2 from Electricity Usage:**
   1. Estimate for compressors, heat exchangers, pumps, and ASU using assumed power consumption metrics
      1. Compressors: 0.6 kWh per kg NH3
      2. ASU (Air Separation Unit): 0.3 kWh per kg NH3
      3. Cooling/Condensation + Others: 0.2 kWh per kg NH3
      4. Total: 1.1 kWh per kg NH3
   2. 8.332044 kg/s NH3 is being produced, so hourly production is:
      1. 8.332044 kg/s x 3600 = 29,995.36 kg/h
   3. Estimated electricity consumption:
      1. 29,995.36 kg/h x 1.1 = 32,994.9 kWh/h
   4. Emission Factor for Electricity:
      1. Assuming a global average: 0.475 kg CO2/kWh (varies by country)
         1. 32,994.9 kWh/h x 0.475 = 15,172.58 kg CO2/h
            1. Convert to kg/s

15,172.58/3600 = 4.2146 kg/s

1. **Total Carbon Footprint**
   1. SMR + Electricity (all) = 143.85 + 4.21 = 148.06 kg/s
2. **Final Output**
   1. Estimated total CO2 Emissions: 148.06 kg/s
   2. NH3 Production Rate: 8.33 kg/s
   3. Carbon Intensity: 17.77 kg CO2/kg NH3

**Step 4: Compare with Green Ammonia Production (Via Electrolysis + Renewable Energy)**

* 1. Hydrogen Source: Electrolysis
  + Reaction:
    - 2H2O → 2H2 + O2
  + Produces H2 using renewable electricity (no fossil fuels)
  + Energy Needed for H2:
    - ~50 kWh of electricity required per kg of H2
    - ~0.178 kg H2 needed per 1 kg of NH3 (from stoichiometry)
    - So:
      * 50 x 0.178 = 8.9 kWh per kg NH3
* 2. Additional Power for ASU, Compressors, etc.
  + ~1.1 kWh/kg NH3 (same as in gray process)
  + Total electricity use = 10 kWh/kg NH3
* 3. Carbon Emissions
  + If powered by 100% renewable energy (solar, wind, hydro):
    - CO2 emissions = 0 kg/kWh
      * Net CO2 = 0 kg CO2/kg NH3
  + If partially powered by grid mix:
    - e.g., 50% renewables, 50% average grid (0.475 kg CO2/kWh)
      * Emissions = 10 kWh x 0.475 x 0.5 = 2.375 kg CO2/kg NH3
* Comparison Summary:

|  |  |  |
| --- | --- | --- |
| * **Category** | * **Gray NH3 (SMR)** | * **Green NH3 (Electrolysis)** |
| * **Energy Source** | * Natural Gas | * Renewable Electricity |
| * **Carbon Intensity** | * 17.77 kg CO2/kg | * 0 – 2.4 kg CO2/kg |
| * **H2 Source** | * CH4 via SMR | * Water Electrolysis |
| * **CO2 Emissions (kg/s)** | * 148.06 | * 0 (ideal) – 19.8 (partial) |
| * **Renewable-ready?** | * No, Fossil-based | * 100% Renewable Possible |

* Takeaways:
  + Green ammonia can reduce carbon emissions by up to 100%
  + It requires ~10x more electricity than gray NH3, but if from renewables, it’s nearly carbon-free
  + Cost and infrastructure are main barriers today

**Step 5: Visualize the Data**

**A graph showing different colored bars

AI-generated content may be incorrect.**

**Step 6: Suggestions For Further Research**

* Life Cycle Assessment (LCA) of Ammonia
* Techno-Economic Analysis (TEA) of Green Ammonia
* Regional Feasibility Mapping
* Dynamic Simulation of Ammonia Production
* Application of Ammonia as an Energy Carrier
* Policy & Carbon Pricing Impact Study