ChemE 486

L1 Simulation

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Simulation

A screenshot of a cell phone

Description automatically generated

**Figure 1.** Block flow diagram

![A close up of a map

Description automatically generated]()

**Figure 2.1** Aspen flowsheet of entire process

![A picture containing clock

Description automatically generated]()

**Figure 2.2** Aspen flowsheet of pressure swing adsorption (PSA) process

![A screenshot of a cell phone

Description automatically generated]()

**Figure 2.3** Aspen flowsheet of electrolysis process

![A close up of a map

Description automatically generated]()

**Figure 2.4** Aspen flowsheet of small-scale Haber-Bosch process

We encountered a warning in the Haber-Bosch process’s reactor (R-101) section, and we will attempt to fix it in L2 simulation. This is due to the recycle stream (stream 18/19). We tried many different approaches such as increasing tolerance, increasing convergence iterations, using a fake purge stream, and more but we couldn’t fully resolve the warning.

\*Note: our simulation will not converge if you reset it! This is a weird quirk of Aspen we encountered.

![A screenshot of a social media post

Description automatically generated]()

**Figure 3.** Warning status in R-101

Meeting Problem Specifications

Our current ammonia production rate is at 435 kg/hr (Stream 17). Since our problem statement require us to produce 50 metric tons per day (50000 kg/day) of anhydrous ammonia at above 99.5 wt% purity, we decide to implement parallel plants to meet the production rate. Our current production rate is at 10,440 kg/day, so we will build 5 parallel plants to meet the specification. Since we used a “magic separator” in the recycle stream to help us achieve convergence without error, we are currently achieving 100 wt% purity. We will remove the “magic separator” for the L2 simulation and will further decide if our plant can meet purity specifications. We achieved a purity of 99.8% without the fake separator.

Stream Table

**Table 1.1** Stream 1-7 from ASPEN Simulation Result

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Stream #** | **Unit** | **1** | **2** | **3** | **4** | **5** | **6** | **7** |
| Water | Kmol/hr | 0.2 | 0.2 | 0.2 | 0.0 | 0.2 | 0.0 | 0.0 |
| Hydrogen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Nitrogen Gas | Kmol/hr | 13.9 | 13.9 | 13.9 | 13.9 | 0.0 | 13.7 | 0.1 |
| Oxygen Gas | Kmol/hr | 3.8 | 3.8 | 3.8 | 3.8 | 0.0 | 0.1 | 3.7 |
| Argon | Kmol/hr | 0.1 | 0.1 | 0.1 | 0.1 | 0.0 | 0.0 | 0.1 |
| Ammonia | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Total Flow | Kmol/hr | 18 | 18 | 18 | 18 | 0 | 14 | 4 |
| Total Flow | Kg/hr | 519 | 519 | 519 | 515 | 4 | 387 | 128 |
| Total Flow | L/min | 7182 | 1893 | 952 | 946 | 0 | 736 | 211 |
| Temperature | C° | 15.0 | 332.5 | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 |
| Pressure | Bar | 1.0 | 8.0 | 8.0 | 8.0 | 8.0 | 8.0 | 8.0 |
| Vapor Frac |  | 1.00 | 1.00 | 0.99 | 1.00 | 0.00 | 1.00 | 1.00 |

**Table 1.2** Stream 8-14 from ASPEN Simulation Result

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Stream #** | **Unit** | **8** | **9** | **10** | **11** | **12** | **13** | **14** |
| Water | Kmol/hr | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.0 |
| Hydrogen Gas | Kmol/hr | 344.1 | 344.1 | 344.1 | 305.4 | 305.4 | 305.4 | 0.0 |
| Nitrogen Gas | Kmol/hr | 244.7 | 244.7 | 244.7 | 230.9 | 230.9 | 230.9 | 0.0 |
| Oxygen Gas | Kmol/hr | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.1 | 0.0 |
| Argon | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Ammonia | Kmol/hr | 0.3 | 0.3 | 0.3 | 26.2 | 26.2 | 26.2 | 26.0 |
| Total Flow | Kmol/hr | 589 | 589 | 589 | 563 | 563 | 563 | 26 |
| Total Flow | Kg/hr | 7557 | 7557 | 7557 | 7537 | 7537 | 7537 | 443 |
| Total Flow | L/min | 32355 | 16350 | 18001 | 19190 | 17636 | 11647 | 1748 |
| Temperature | C° | 121.5 | 321.5 | 382.0 | 460.0 | 399.0 | 170.0 | 400.0 |
| Pressure | Bar | 10.0 | 30.0 | 30.0 | 30.0 | 30.0 | 30.0 | 13.8 |
| Vapor Frac |  | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 | 1.00 |

**Table 1.3** Stream 15-21 from ASPEN Simulation Result

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Stream #** | **Unit** | **15** | **16** | **17** | **18-1** | **19** | **20** | **21** |
| Water | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 39.0 | 51.6 |
| Hydrogen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 305.4 | 305.4 | 0.0 | 0.0 |
| Nitrogen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 230.9 | 230.9 | 0.0 | 0.0 |
| Oxygen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.1 | 0.0 | 0.0 | 0.0 |
| Argon | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Ammonia | Kmol/hr | 26.0 | 0.5 | 25.5 | 0.3 | 0.3 | 0.0 | 0.0 |
| Total Flow | Kmol/hr | 26 | 1 | 26 | 537 | 537 | 39 | 52 |
| Total Flow | Kg/hr | 443 | 8 | 435 | 7094 | 7089 | 703 | 929 |
| Total Flow | L/min | 26 | 14 | 12 | 11119 | 10113 | 12 | 16 |
| Temperature | C° | 32.0 | 32.0 | 32.0 | 170.0 | 130.0 | 15.0 | 19.9 |
| Pressure | Bar | 13.8 | 13.8 | 13.8 | 30.0 | 30.0 | 1.0 | 1.0 |
| Vapor Frac |  | 0.02 | 1.00 | 0.00 | 1.00 | 1.00 | 0.00 | 0.00 |

**Table 1.4** Stream 22-28 from ASPEN Simulation Result

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Stream #** | **Unit** | **22** | **23** | **24** | **25** | **26** | **27** | **28** |
| Water | Kmol/hr | 51.6 | 51.6 | 2.5 | 10.4 | 2.5 | 0.1 | 2.4 |
| Hydrogen Gas | Kmol/hr | 2.5 | 2.5 | 41.2 | 0.0 | 41.2 | 41.2 | 0.0 |
| Nitrogen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Oxygen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 19.3 | 0.0 | 0.0 | 0.0 |
| Argon | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Ammonia | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Total Flow | Kmol/hr | 54 | 54 | 44 | 30 | 44 | 41 | 2 |
| Total Flow | Kg/hr | 934 | 934 | 128 | 806 | 128 | 85 | 43 |
| Total Flow | L/min | 1037 | 2140 | 21369 | 14514 | 18450 | 1184 | 1 |
| Temperature | C° | 19.7 | 80.0 | 80.0 | 80.0 | 35.0 | 35.0 | 35.0 |
| Pressure | Bar | 1.0 | 1.0 | 1.0 | 1.0 | 1.0 | 15.0 | 15.0 |
| Vapor Frac |  | 0.05 | 0.08 | 1.00 | 1.00 | 0.99 | 1.00 | 0.00 |

**Table 1.5** Stream 29-33 from ASPEN Simulation Result

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Stream #** | **Unit** | 29 | 30 | 31 | 32 | 33 |
| Water | Kmol/hr | 0.1 | 0.0 | 10.4 | 0.2 | 10.2 |
| Hydrogen Gas | Kmol/hr | 38.7 | 2.5 | 0.0 | 0.0 | 0.0 |
| Nitrogen Gas | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Oxygen Gas | Kmol/hr | 0.0 | 0.0 | 19.3 | 19.3 | 0.0 |
| Argon | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Ammonia | Kmol/hr | 0.0 | 0.0 | 0.0 | 0.0 | 0.0 |
| Total Flow | Kmol/hr | 39 | 2 | 30 | 20 | 10 |
| Total Flow | Kg/hr | 80 | 5 | 806 | 622 | 184 |
| Total Flow | L/min | 1113 | 71 | 8664 | 1661 | 3 |
| Temperature | C° | 35.0 | 35.0 | 35.0 | 35.0 | 35.0 |
| Pressure | Bar | 15.0 | 15.0 | 1.0 | 5.0 | 5.0 |
| Vapor Frac |  | 1.00 | 1.00 | 0.68 | 1.00 | 0.00 |

References

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Minnesota (relative) humidity:

High: 80.7%

Low: 59.8%

Assume average humidity: 70%

Source: <https://www.dnr.state.mn.us/faq/mnfacts/climate.html>

Calculator: <https://www.rotronic.com/en-us/humidity_measurement-feuchtemessung-mesure_de_l_humidite/humidity-calculator-feuchterechner-mr>