

The ChemSep/COCO Casebook: Air Separation Unit

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The objective of this article is to describe the modeling of an air separation unit using the (free) flowsheeting system known as COCO (van Baten et al., CACHE News, Fall, 2006), and **ChemSep™**.

The cryogenic air separation process shown in Figure 1 involves the tight integration of heat exchangers and separation columns that is completely driven by the compression of the air at the inlet of the unit. The air inlet stream is cooled and partially liquefied against the leaving product streams. Nitrogen is then separated at a pressure of 6 bar in the first column and condensed against boiling oxygen at a lower pressure (around 1.2 bar). These two columns share the same column shell to minimize the temperature difference between the condensing nitrogen and evaporating oxygen. The liquid bottom product of the high pressure column is rich in oxygen and is reduced in pressure. The Joule-Thomson (JT) effect cools this rich liquid such that it can be used to run the condenser of a side rectifier that separates argon from oxygen. This side rectifier is fed with a vapor side draw from the low pressure column. The whole process requires additional cooling which can be obtained using an expander that feeds compressed air directly to the low pressure column. Thus, a certain part of the air cannot be separated but leaves the unit as a waste stream. Gaseous nitrogen and oxygen, and liquid argon are the products. With temperature differences in the heat exchangers of just a few degrees Kelvin; clearly there is a significant interaction in these interconnected columns when any of the manipulated variables are adjusted or when a disturbance affects one of the column controlled variables. Purities in nitrogen and argon are typically very high, with 1 ppm or less impurities. The oxygen product purity ranges from 97.5 to 99.5%.

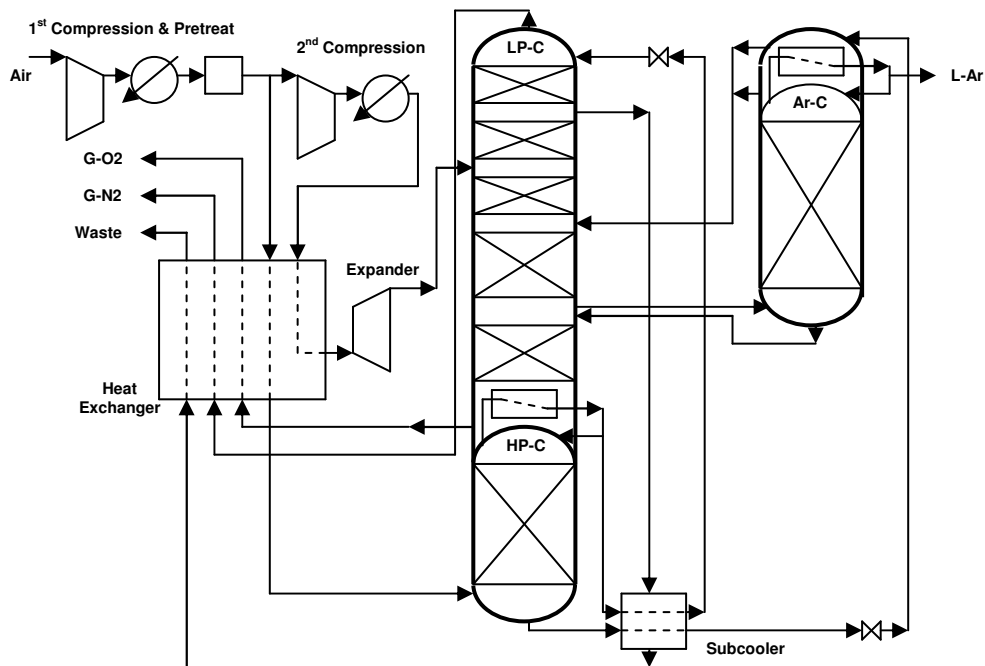


Figure 1: Flowsheet of air separation unit.

The stream table for the low pressure column is shown in Figure 5

| Stream | Feed3 | Feed6 | Feed1 | Feed5 | |
|---------------------|------------|------------|------------|------------|------------|
| Stage | 1 | 15 | 20 | 20 | |
| Pressure (bar) | 1.30000 | 1.30000 | 1.29773 | 1.29773 | 1.30000 |
| Vapour fraction (-) | 0.119777 | 1.00000 | 2.8496E-04 | 1.00000 | 0.00000 |
| Temperature (K) | 79.6333 | 96.2938 | 82.5399 | 82.5399 | 92.0000 |
| Enthalpy (J/kmol) | -1.085E+07 | -5.918E+06 | -1.229E+07 | -6.328E+06 | -1.260E+07 |
| Entropy (J/kmol/K) | 230961 | 167312 | 249892 | 161571 | 910000 |
| Mole flows (mol/s) | | | | | |
| Nitrogen | 841.842 | 404.635 | 938.205 | 512.888 | 1.006E+06 |
| Oxygen | 5.9316E-07 | 108.514 | 535.039 | 79.8752 | 2.000E+05 |
| Argon | 5.8929E-04 | 4.81708 | 22.4561 | 4.84008 | 1.600E+05 |
| Total molar flow | 841.843 | 517.966 | 1495.70 | 597.604 | 2.100E+06 |
| Mole fractions (-) | | | | | |
| Nitrogen | 0.999999 | 0.781200 | 0.627268 | 0.858241 | 4.612E-01 |
| Oxygen | 7.0459E-10 | 0.209500 | 0.357718 | 0.133659 | 0.900E-01 |
| Argon | 7.0000E-07 | 0.00930000 | 0.0150138 | 0.00809915 | 0.070E-01 |
| Mass flows (kg/s) | | | | | |
| Nitrogen | 23.5834 | 11.3354 | 26.2829 | 14.3681 | 2.820E+05 |
| Oxygen | 1.8980E-08 | 3.47234 | 17.1207 | 2.55593 | 6.400E+04 |

Figure 5: Screenshot of ChemSep stream table for the low pressure column in ASU.

The composition flow profiles in the low pressure column are shown in Figure 7. The internal flow rates in the LP column must vary so as to obtain a pure gaseous nitrogen top product as well as reasonably pure oxygen in the bottoms. At the same time the vapor draw from the LP column to the argon column must be low enough in nitrogen to prevent buildup of N₂ in the argon column, yet high enough in argon for the argon column not to become pinched.

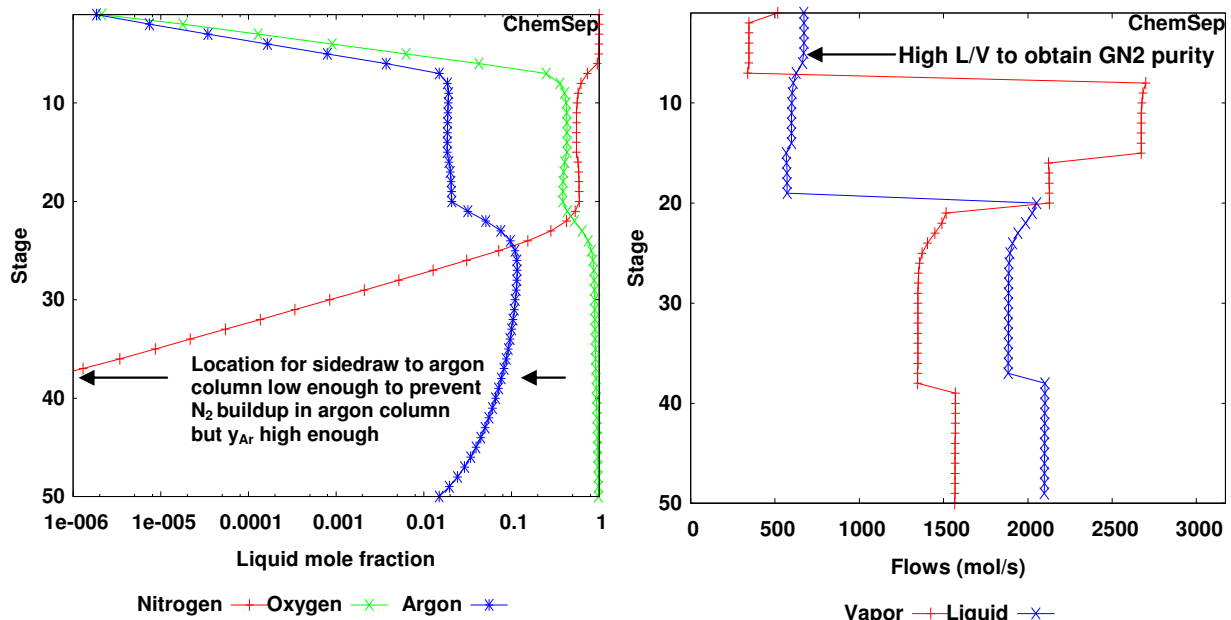


Figure 6: Composition and flow profiles in the low pressure column in ASU.

The McCabe-Thiele diagrams displayed by ChemSep (shown in Figure 7) let the modeler quickly evaluate the process and the feed and draw locations to/from the low pressure column.

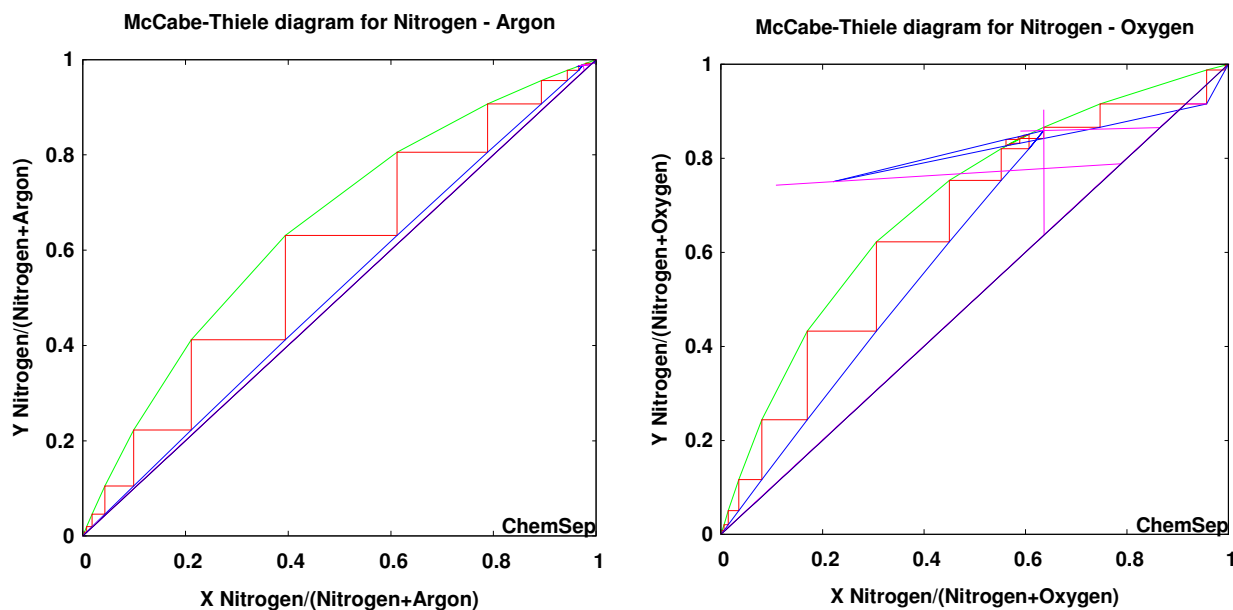


Figure 7: McCabe-Thiele diagrams for low pressure column in ASU.

Availability:

COCO is freely available from <http://www.cocosimulator.org/>.

ChemSep-Lite is included in the COCO installation program, and also is freely available from <http://www.chemsep.com/>. The full version of **ChemSep** is available for educational use from the CACHE corporation (<http://www.cache.org/>).

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