## 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<sup>™</sup>**.

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.

In the simplified process shown in Figure 2 the second compression stage and the sub-cooler are omitted at the expense of lower recoveries. This is the version of the ASU that will be modeled using COCO.



Figure 2: Simplified air separation unit

Figure 3 shows a screenshot of the simplified ASU as set up in COCO. This flowsheet was simulated with one tear stream: the liquid stream 22 from the argon column (Ar-C) back to the low pressure column (LP-C). Normally, the argon column bottoms liquid flows back to the low pressure column by means of gravity. This is simulated by using a pump that raises the pressure of the bottoms liquid, as otherwise COCO warns us that the bottom's liquid would flow against a pressure gradient (the argon column operates at a lower pressure than the low pressure column). Also, note that there is a vapor and a liquid drawn from the condenser of the high pressure column reboiler duties to be matched by a controller. The combined stream is fed to the top of the low pressure column (via a separator). The rich liquid bottom product of the high pressure column is flashed. Here, the heat input is set equal to the condenser duty of the argon side rectifier. The gaseous product streams are heated up against the inlet air flow to recover heat.

The 3 distillation columns in the COCO flowsheet are modeled using ChemSep. All other units (the heat exchangers, valves, and flashes) are from the COUSCOUS unit operations package in COCO.

The specifications made on the various unit operations of the ASU are shown in Figure 4. As the number of stages in ChemSep LITE is limited to 50, the obtainable purities for the liquid argon at the top of the side rectifier and of the oxygen in the low pressure column are less than what they normally are. Nowadays, using structured packing, it is possible to equip the argon column with enough stages to reduce the impurities to less than 1 ppm. Note that we included heat leaks into the columns from the environment as well as pressure drops in the columns over the column internals, which raises the required inlet pressure for the ASU.



Figure 3: ASU in COCO showing plant specifications

Heat integration for the ASU is shown in Figure 4. The cooling of the feed is used against the product streams in the main heat exchanger, the LP condenser against the HP reboiler, and the condensation of argon against the vaporization of rich liquid.



Figure 4: Heat integration in ASU

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

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Title Components Operation Properties Thermodynamic:	Tables Graphs McCabe-Thiele Tables Select table: Streams		XL Edit	Сору	Font Print	
Reactions	Stream	Feed3	Feed6	Feed1	Feed5	
Feeds Specifications Analysis Pressures Heaters/Coolers 	Stage Pressure (bar) Vapour fraction (-) Temperature (K) Enthalpy (J/kmol) Entropy (J/kmol/K)	1 1.30000 0.195777 79.6333 -1.085E+07 230961	15 1.30000 1.00000 96.2938 -5.918E+06 167312	20 1.29773 2.8496E-04 82.5399 -1.229E+07 249892	20 1.29773 1.00000 82.5399 -6.328E+06 161571	1.: 0.00 92 -1.26: 91:
✓ Sidestreams ✓ Column specs ⊡ ✓ Results	Mole flows (mol/s) Nitrogen Oxygen Argon	841.842 5.9316E-07 5.8929E-04	404.635 108.514 4.81708	938.205 535.039 22.4561	512.888 79.8752 4.84008	1.006: 20: 16
Graphs	Total molar flow	841.843	517.966	1495.70	597.604	21;
McCabe-Thiele Units Solve options Paths	Mole fractions (-) Nitrogen Oxygen Argon	0.9999999 7.0459E-10 7.0000E-07	0.781200 0.209500 0.00930000	0.627268 0.357718 0.0150138	0.858241 0.133659 0.00809915	4.612: 0.9: 0.07:
	Mass flows (kg/s) Nitrogen Oxygen	23.5834 1.8980E-08	11.3354 3.47234	26.2829 17.1207	14.3681 2.55593	2.820 6. <del>-</del>
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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://<u>www.chemsep.com</u>/. The full version of *ChemSep* is available for educational use from the CACHE corporation (http://<u>www.cache.org</u>/).

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