McMaster University ENGINEERING

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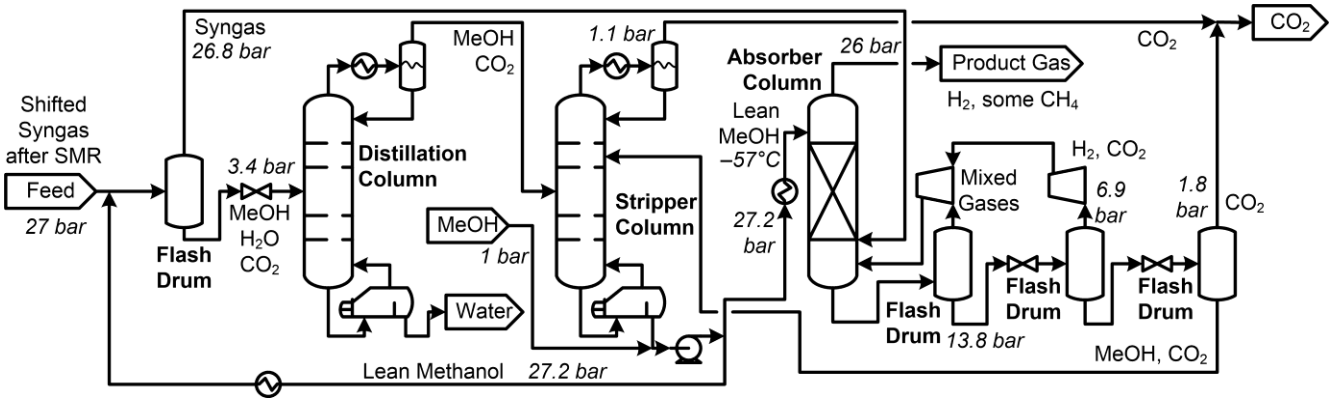
Overview

- **Primary feed**: Shifted syngas from steam methane reforming. About 75% H_2, 19% CO_2, with the balance unreacted CH_4, CO, N_2, and leftover water remaining from an upstream condensing step.
- **Solvent**: Methanol
- **Pressure**: 27 bar absorber. 1.1 bar stripper.
- **Capture CO_2 Conditions**: 1 bar, >98 mol% purity, -79°C
- **Energy Consumption**: Very high
- **Scale**: 111 tonne/hr shifted syngas feed.
- **Optimization**: Not optimized.
- **Intended use**: Education and demonstration

Process



The Rectisol process, shown above[1], uses methanol as the primary solvent. The syngas to clean is first dewatered by mixing it with cold methanol (about -21°C). This is appropriate for use after condensation has been used to recover most of the water, but there is still water remaining to remove. Some CO2 will be captured with this water in the liquid phase as well. This uses about 60 mol of methanol for each mol of water removed in this drum, but this can be adjusted. The more you have, the more water you capture (which is desired), but the more CO2 you also capture (which is not desired, since it will put additional load on the distillation column).

The shifted syngas that leaves the drum has been dewatered but still has much CO2 to capture. This is sent to the bottom of the absorber column. This uses 10 absorber stages, but this is subject to optimization. The column should still be at high pressure, basically, the pressure of the original shifted syngas feed, just a little lower because of pressure drop. The lean (pure) methanol feed at the top of this column is best between 11.7 to 12 mole of methanol per mol of CO2 that will be absorbed in the column. Again, this can be adjusted for optimization purposes. The gas leaving this column should only have small amounts of CO2 left, and almost all of the other gases, especially hydrogen.

The liquid methanol leaving the bottom of the absorber will contain the captured CO2. To get it out of the solvent, a flash cascade is used. High pressure drums have some H2 so it is recycled to the absorber via compressors.

[1] The modelling strategy was adapted from Adams TA II, Khojestah Salkuyeh Y, Nease J. Processes and Simulations for Solvent-based CO2Capture and Syngas Cleanup. Chapter in: Reactor and process design for in sustainable energy technology. Elsevier (2014). Pages 163-232. ISBN: 978-0-444-59566-9. The process was based on a similar process for IGCC from Doctor RD, Molburg JC, Thimmapuram PR, Berry GF, Livengood CD. Gasification combined cycle: carbon dioxide recovery, transport, and disposal. US DOE Report, Argonne National Laboratory ANL/ESD-24. 1994.

Tom's Tips

When modelling the absorber with RadFrac, convergence can be greatly helped by setting the Absorber parameter to "Yes" in the blocks' Convergence | Convergence | Advanced form.

Also, once you have something to converge in any form, use the generate estimates feature to record the results to be estimates for future runs, especially temperature and mole fraction data. This is true of all columns. This will make future changes much easier to accomplish because when you reinitialize, you'll use these results as the initial guesses for the run.

The liquid leaving the dewatering flash drum is purified by distillation, to recover the methanol, and get the water out. A classic distillation column with a vapor product works well. 16 to 20 stages is about right, with the feed about halfway. A reflux ratio on the order of 220 (because the water content is so low) and a reboil ratio on the order of 2.2 should work. These are subject again to optimization. They key thing is to get high purity water out of the bottom, and the rest of the CO_2 out with the methanol in the vapor phase.

Finally, the loaded methanol streams need to be purified in the stripper. The key goal here is excellent separation, with high purity (at least 95 mol%) CO_2 in the distillate, and very high purity (99.9 mol%) methanol in the bottoms. The boilup ratio can be low (around 1) but the reflux ratio may need to be as high as 20. About 19-20 stages is about right with the feed at stage 17 or lower. However, this is definitely subject to optimization.

The distillation column and stripper have very large energy consumption requirements, especially the stripper which requires a very cold refrigerant in the partial condenser.

This one is usually the hardest to get to converge. The best approach is usually to get *something* to converge, use generate estimates, and then slowly change the parameters until you get something you like, using generate estimates again and again as you go with each successful run, with lots of saving. I find that convergence is easier when the reflux ratios are higher than you want, and then you sort of walk it down to where you want it to go.

Finally, the lean methanol (the bottoms product) will need to be pumped and cooled again so it can be recycled to the absorber or dewatering flash drum. The stream immediately after the pump is used as the tear stream. A calculator block is used to provide the correct methanol makeup stream, which should be small. In the event that it is not small, it usually means the distillation column has undesired methanol in its water product.

Citation
Please cite this model as:

Adams TA II. Aspen Plus Simulation of a Rectisol Process for Blue Hydrogen Production. LAPSE:2021.0100

Updates
Find the most recent version of this model at http://PSEcommunity.org/LAPSE:2021.0100