Chemcad Training Manual

Recovery of Crude Acrylonitrile (ACRYLO3A)

Introduction

The binary system acrylonitrile (bp 77.7°C) and acetronitrile (bp 81.°C) are relatively ideal and thus difficult to separate by conventional distillation. However, in the presence of water, the relative volatility of acrylonitrile relative to acetronitrile is approximately tripled. Acrylonitrile and water form a hetergeneous azeotrope because this system is only partially miscible. The aqueous solution from the Absorber Bottom is fed to the middle of the Recovery Column and this column operated to make the split between these components. Water is fed up to the top of the column to enhance the separation. Stripping of acrylonitrile occurs in the bottom of the column: rectification of acetonitrile and acrylonitrile occurs in the top of the column. The column overhead vapor is condensed. The aqueous layer is returned to the middle of the column; the organic layer is taken as product. The vapor rate to the bottom of the column is sufficiently high so that only one liquid phase (the aqueous phase) is present on the trays of this column. Hydrogen cyanide as well as the other organics produced in small quantities leave the system at this point.

Bottoms from the Recovery Column are fed to the Stripper Column where <u>both</u> acrylonitrile and acetonitrile are stripped. There is no attempt made to prevent acrylonitrile in the Recovery Column bottoms from going overhead in the stripper. Indeed the ratio of acrylonitrile to acetonitrile in the overhead is somewhat greater than in the feed. A vapor sidestream is taken near the top of the column. The vapor contains nearly 15-20 wt% acetonitrile and is used to heat the Recovery Column. The top of the Stripper serves to concentrate both acrylonitrile and acetonitrile.

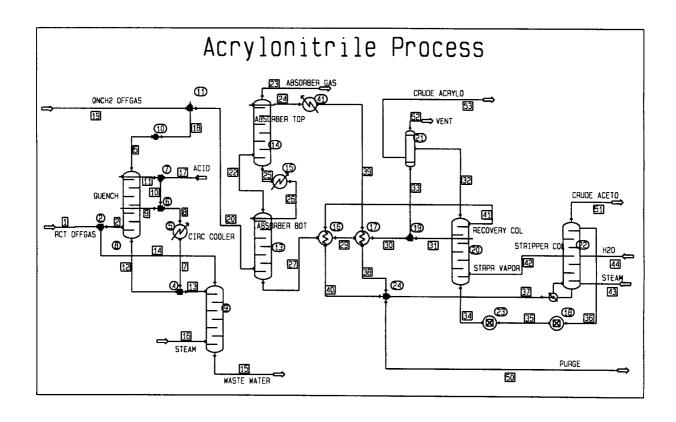
Simulation

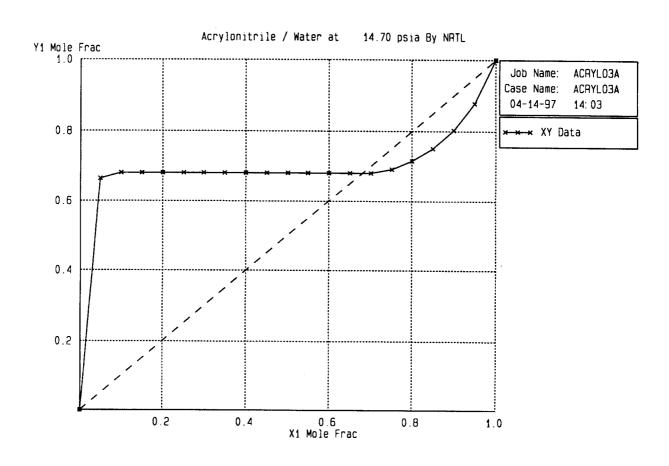
The simulation is best carried out in a step-wise manner. The Quench Column was simulated first. Streams 9, 10, and 14 were selected as the cut streams in this part of the flowsheet. It was initially assumed that these three streams were 100% water. The outlet temperature of the Circulation Cooler (Item 5) was fixed at 41oC, about the lowest temperature practical with cooling water. Stream 7 was fixed at 41oC, about the lowest temperature practical with cooling water. Stream 7 was fixed at 3.444E6 lbs/hr; Stream 10 was fixed at 730,000 lbs/hr. This combination gave a reasonable amount of waste water (Stream 15). After the composition and amount of Stream 13 was determined by simulation of the Recovery Column, Tower 9 (Stripper) was simulated. It was then feasible to simulate both columns at once.

After the Quench part of the flowsheet was complete, the amount and Composition of Stream 20 was known. It was initially assumed that the scrubbing water to Absorber Top and the liquid from Absorber Top to Absorber Bottom were both pure water. The amount of scrubber liquid was determined in preliminary process calculations. With these assumptions, the Absorber system was simulated. The amount and composition of Stream 12 (vapor to base of Recovery Column) was fixed as well as the composition of Stream 33, permitting simulation of the Recovery Column. Finally, the Stripper Column alone was simulated.

With all of this work completed, the entire flowsheet could be simulated with confidence. Initially, Controllers 18 and 23 were turned off to give added stability. When a solution to the whole flowsheeet was detained, the controllers were turned on to give the desired specifications in the Recovery Column and Stripper Column.

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Acrylonitrile Recovery

The recovery of acrylonitrile from reactor offgas is a complex process. This system provides a good example of how to simulate a highly non- ideal, multi-component system. The compositions of the reactor off-gas, absorber gas, crude acrylonitrile and crude acetonitrile are given in the table below. There are two reactors, two identical Quench Systems (only one shown) and one combined recovery system.

Absorber Top/Bottom

The mixture of gases from the two Quench Systems is fed to the base of the Absorber Bottom. Water is fed to the Absorber Top. Essentially all of the fixed gases (oxygen, nitrogen, carbon monoxide, and carbon dioxide) leave the Absorber Top. Most of the acrylonitrile and other organics are absorbed.

Quench Column and Stripper

The purpose of the Quench System is to remove all of the fixed gases and a large part of the contained water vapor, as well as to cool the reactor product. Contained ammonia is converted to ammonium sulfate by reaction with sulfuric acid. The ammonium sulfate that is formed is removed as a dilute solution from the base of the Quench Stripper.

Stream No.	1	23	51	53
Stream Name	React Prod	Tail Gas	Crude Aceto	Crude Acrylo
Water	1954	1440	73.0	435.1
Acrylonitrile (bp 77.7°C)	412.3	5.95	.840	815
HCN (bp 26°C)	141.7	7.30	4E-4	270
Acetonitrile (bp 81.6°C)	16.06	.95	30.1	.80
Propionitrile (bp 97.3°C)	.50	3E-5	.070	.93
Acetone (bp 56.5°C)	.3	2E-5	.014	.58
Acrolein (bp 52.69°C)	15.8	9.89	7E-7	21.5
Nitrogen	5500	11000	0	
.0007				
Oxygen	48.5	97.0	0	3E-5
Carbon Monoxide	104	208	0	3E-5
Carbon Dioxide	189	343.9	0	20.9
Propane	25.0	19.4	5E-5	27.9
Propylene	12.7	12.6	4E-7	11.5
Ammonia	19.9	.009	3e-11	.012
Sulfuric Acid	0	0.0	0	0
(NH ₄) ₂ SO ₄	0	0.0	0	0
HEAVY	1.0	3E-14	6E-16	5E-13