**MEMORANDUM** \_

Date: April 9th, 2013

To: Dr. El-Halwagi

From: Alejandra Europa Casanueva

Re: Workshop #10 (Merging Simulation Files)

**Introduction**

This workshop was aimed to learn how to merge two APEN Plus files. For this workshop, a RSTOIC reactor and a RADFRAC column were merged with the purpose of using the distillate product of the distillation column as feed for the reactor. The column has 46 stages including the total condenser and the reboiler. The column operates at 18 psia, and has a stage drop of 0.1 psi. A water/methanol feed is introduced to the column. The two blocks are linked by using the distillate product in the column as methanol feed to the reactor. The reactor is used to form methyl acetate by reacting acetic acid and methanol\*. The reactor operates at 330 K and 1 atm, with a 60% methanol conversion.

\*CH3CO2H + CH3COH 🡪 CH3CO2CH3 + H2O

Acetic Acid + Methanol 🡪 Methyl Acetate + Water

**Objectives**

1. Merge the two ASPEN Plus Files and link the two blocks. Determine the composition of the product form the reactor.
2. Use this process to develop a method to obtain a product stream with more than 75 wt% methyl acetate. This method should also recycle all the unreacted acetic acid, and at least 25% of the unreacted methanol, back to the reactor. Modify the process by adding up to two additional separation units

**Conclusions**

1. The first task was to link the two processes by using the distillate of the distillation column as the methanol feed to the reactor (see Figure 1). Table 1 shows the composition of the product stream from the reactor, which is approximately 50 wt%.



**Figure 1. The Merged Distillation-Reactor Process**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Component | Mole Flow (lbmol/hr) | % Composition | Mass Flow (lb/hr) | % Composition (WT) |
| Water  | 1286.797 | 0.422 | 23162.346 | 0.185 |
| Methanol | 561.7296 | 0.184 | 17997.816 | 0.144 |
| Acetic Acid | 356.3553 | 0.117 | 21399.136 | 0.171 |
| Methyl Acetate | 842.5944 | 0.276 | 62419.393 | 0.499 |
| Total  | 3047.4763 | 1.000 | 124978.691 | 1.000 |

**Table 1. Composition of the product from the reactor**

1. The second task was to find a way to get a product stream with at least 75 wt% methyl acetate. In order to do this, another distillation column having 40 stages (including condenser and reboiler) was added to the process (see Figure 2). The column has a reflux ratio of 1.4, a distillate rate of 60,000 lb/hr, and an operating pressure of 1 atm. The reactor product is introduced to the column above stage 26. The split fractions in the product streams of the new column are shown in Figure 3. It can be seen that the main product stream (1) contains more than 75wt% methyl acetate, and that all the unreacted acetic acid and at least 25% of the unreacted methanol is being recycled back into the reactor.



**Figure 3. Split Fractions for the added column**



**Figure 2. Flowsheet of new synthesized process with recycle.**

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Component | Mole Flow (lbmol/hr) | % Composition | Mass Flow (lb/hr) | % Composition (WT) |
| Water  | 20.64281 | 0.022 | 371.57058 | 0.006 |
| Methanol | 192.0567 | 0.206 | 6153.497 | 0.103 |
| Acetic Acid | 3.3689E-21 | 0.000 | 0.000 | 0.000 |
| Methyl Acetate | 721.8493 | 0.772 | 53474.596 | 0.891 |
| Total  | 934.54881 | 1.000 | 59999.663 | 1.000 |

**Discussion**

The original process, which only incudes the distillation column and the reactor, results in a poor composition of the product. The product stream consists of 50 wt% methyl acetate (desired product), and the rest is water, and unreacted methanol and acetic acid. In order to obtain a more pure stream and to optimize the process, another distillation column was added to separate the methyl acetate from the other components. Through this new column, it was possible to achieve a product stream consisting of 89% methyl acetate. The bottoms product, which contained water, methanol and acetic acid, was recycled back into the reactor. This process ensured that all the unreacted acetic acid was reused and that at least 25% of the unreacted methanol was also recycled. Through this simulation, it was learned how to merge two simulations, and to create a system that separates, reacts, and recycles.

**Recommendations**

Another separation unit could be added to achieve a higher weight percent composition in the final product stream. The addition of a second separation unit might also result in a higher amount of methanol being recycled. Recycling unused reactants is important to reduce the amount of fresh materials needed. Also, sensitivity analysis could be used to find the most energy efficient distillation column(s), by varying the number of stages and feed entry.