INTEGRATED CHEMICAL ENGINEERING SOFTWARE – POWER AND SPEED

Tightly integrated software packages now make it possible for chemical engineers to perform more realistic and detailed analysis than they have ever done before, and do it in record time. The result is better designs from both the cost and operational standpoint. Below a very brief example and overview of some the more important steps and features of these tools is by way of explanation.

For our example process let us take the dehydration of ethanol via azeotropic distillation using n-pentane as the entrainer. For simplicity's sake we'll focus on the dehydration column (and its associated equipment) only. Thus, we are looking at the following flowsheet.



The feed is ethanol and water at the azeotrope.

The n-pentane, introduced at the top of the column, forms a heterogeneous, minimum boiling, ternary azeotrope with the water and ethanol. The minimum boiling azeotrope goes to the top of the column carrying the water with it. The vapor coming off the top tray (before entering the condenser) is very close in composition to this azeotrope. When this vapor is condensed, it splits into two liquid phases. The organic phase is refluxed and the aqueous phase is decanted (as tops product). Pure ethanol comes out the bottom of the columns as product (99.99 mole%).

Step 1: Establish the thermo model.

The first thing we would want to do is accurately establish the thermodynamics. A quick literature search will yield the following facts about this system:

- i. Ethanol and water are miscible and form an azeotrope at 90.4 mole% ethanol and 173.1°F.
- ii. Ethanol and n-pentane are miscible and form an azeotrope at 92.4 mole% pentane and 93.7°F.
- iii. Water and n-pentane are immiscible and form a heterogeneous azeotrope 94.6 mole% pentane and 94.3°F.

iv. The system of mixtures of ethanol, water, and n-pentane has a miscibility gap and form a minimum boiling heterogeneous azeotrope of 4.4 mole% water, 6.1 mole% ethanol, and 89.5 mole% n-pentane at 92.1°F.

Using the CHEMCAD K-Value Wizard, the thermodynamic model NRTL was chosen for this system. CHEMCAD then loaded the component physical properties (stored in the program database) and the phase equilibrium interaction parameters (also stored in the database). A Residue Curve Map and binodal plot were then computed and plotted by the program. The result was as shown below:



Figure 2 Residue Map for EtOH-H2O-nC5 System

From this map we can verify our thermodynamic model.

	Miscible/immiscible	Azeotrope composition, mole%	Azeotrope temperature, F
Ethanol-water	Miscible	90.4 .v. 90.8 EtOH	172.8 .v. 173.1
Ethanol-npentane	Miscible	92.4 .v. 92.2 nC ₅	93.7 .v. 95.5
npentane-water	Immiscible	94.6 .v. 94.6 nC ₅	94.3 .v. 93.8
Ethanol-water-npentane	immiscible	4.4,6.1,89.5 .v. 4.9,5.4,89.7	92.1 .v. 93.2

The above comparison verifies that the chosen thermodynamic model is probably good enough for final design purposes and is easily adequate for calculation at the early stages of a design.

Step 2: Calculate a preliminary material balance around the column

The next step would be reconstruct this map at our selected operating pressure (50 psia) and use it to prepare an initial heat and material balance using this thermo model. Conveniently, the residue map can be used to prepare a fairly accurate material balance around the column.

This is done by selecting a top tray vapor composition which has the following characteristics:

- i. It is located in the same distillation region as the bottom product composition (99.99 mole% ethanol);
- ii. it is located in the three phase region;
- iii. it is far enough into the three phase region so that when it condenses it splits into two liquid phases which straddle the distillation boundaries; but, It is not so far into the three phase region that the top tray liquid (the liquid which is in equilibrium with the top tray vapor) has two liquid phases (which would make it hard to operate).

Figure 3 below illustrates this process with the result shown in Figure 4.



Residue Map for EtOH-H2O-nC5 System

Figure 3

The red lines represent the distillation boundaries or limits.



Figure 4: Preliminary material balance

Step 3: Number of stages

How many "ideal" stages?

The material balance calculated above assumes that we have enough stages to make the separation. We can do a sensitivity analysis on the number of stages to determine how many are needed. The plots below demonstrate the this:



As you can see, in order to reach the desired purity of 99.99% ethanol in the product we need at least 14 stages (including the reboiler, but excluding the condenser). We can further see that from stage 14 on the product recovery is the same. There is therefore no advantage in having more stages. However, the above sensitivity analysis is assumes "ideal" stages in the column; that is, the separation efficiency on each stage is 100%. Obviously this is untrue. As a result we need more than 14 stages. But how many more?

How many actual or real stages?

Separation efficiencies are different for every component on every tray. The efficiencies themselves are function not only of the liquid solution, but also of the mass transfer device (packing, valve trays, sieve trays, etc.) used and the vapor and liquid traffic. An analysis based upon "ideal" stages would need a separation efficiency matrix n components by m stages determined for the exact mass transfer device and flowrate profile, in order to be precisely accurate. Such numbers are not generally available and are rarely used.

A more practical approach is to run the simulation based on a mass transfer approach. The issue of separation efficiency then becomes mute, because the phase equilibrium and the mass transfer resistance are both built directly and explicitly into the calculation. This approach does require specific knowledge of the mass transfer device. This we can get from CHEMCAD by asking it to size and lay out the trays. Assuming valve trays, CHEMCAD calculates the following tray size and layout:

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Tray Loadings	Vapor	Liquid		
	64176.582 lb/h	62944.359 lb/h		
	124535.495 ft3/hr	1723.614 ft3/hr		
Density	0.515 lb/ft3	36.519 lb/ft3		
System factor		1.000		
Valve type : V-1				
Valve material : S.S.				
Valve thickness, gage		12.000		
Deck thickness, gage		14.000		
Tower internal diameter,	It	6.000		
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Weir beight in		2 000		
Flow path length in		50.500		
Flow path width in		65.559		
Tray area, ft2		28.274		
Tray active area ft2		22.991		
% flood		47.900		
Hole area ft2		4.368		
Approx # of valves		342		
Tray press loss, in		3.977		
Tray press loss, psi		0.084		
Dry press drop, in		2.138		
Downcomer clearance in		3.000		
Downcomer head loss in		0.130		
Downcomer backup in		7.205		
Downcomer residence time,	sec	3.313		
Liquid holdup ft3		5.110		
Liquid holdup 1b		186.605		
Design pressure, psia		47.558		
Joint efficiency		0.850	-	
Allowable stress psia		13700.000		
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Figure 6: The tray layout information

Using these column and tray parameters, we can now redo our sensitivity study based on mass transfer or "real" stages the result is given below:



We now see that when mass transfer resistances are accounted for we need at least 18 stages to meet our product specifications. This column was actually built with 19 stages and ran well.

The impact of mass transfer resistances goes far beyond how many stages are required to achieve product purity. Many other issues can be affected. Such issues include temperature profile changes; condenser and reboiler duties; vapor liquid traffic; entrainer requirements; etc., etc. For instance look at the comparison of the temperature profiles when the column is run with 19 stages under "ideal" and "mass transfer" conditions.



You can see the region of temperature change (and therefore composition change) is significantly different, affecting how and where the temperature sensors and control devices are placed and set.

At this stage we can accomplish several things necessary to our preliminary process study. These are:

- i. size the equipment
- ii. resimulate the flowsheet including the effects of equipment sizes on the simulation. Where as our first simulation was an "ideal" simulation (assuming trays and heat exchangers perform <u>exactly</u> as required), this next simulation will be a "real" simulation; that is, including the effects of pressure drops, heat and mass transfer.
- iii. Having the equipment sizes, we can estimate the equipment and installation costs.
- iv. Having the feed and utility rates from the "real" simulation, we can compute a cash flow and present value analysis on the project.

Step 4: THE EFFECT OF EQUIPMENT SIZES AND CONFIGURATIONS ON THE HEAT AND MATERIAL BALANCE

Equipment size and configuration impacts a steady state heat and material balance through three mechanisms; heat transfer, mass transfer and pressure drop resistances. The effect of mass transfer resistances is felt primarily in the distillation column performance. This was addressed above so we will not look closer at it here. The effect of heat transfer resistances primarily effects the performance of heat exchange equipment. This is what we will examine now.

In the CHEMCAD library is a detailed sizing/rating module for heat exchangers. This module calculates pressure drops, film coefficients, and required areas based upon prevailing stream conditions. To make this calculation the inlet and outlet streams must be known in order to determine the heat curve required for the pressure drop and heat transfer analysis. The result is a design which is somewhat under or over design (has a little more or a little less surface area than required) because it has to conform to commercially available sizes. In the real world this excess (deficient) area will be used and will have some impact on plant operations. What is that impact and how do we deal with it?

These issues can be addressed by including the heat transfer and pressure drop calculations directly in the simulation. In this mode the inlet streams and geometry will be inputs to the heat exchanger and the output streams will be computed based upon the HX geometry. In this way the exact effects of the entire exchanger will be accounted for. The flowsheet was modified as shown in Figure 9 using 80°F, 50 psia cooling water. A sensitivity analysis was run varying the cooling water flowrate. The exchanger outlet temperatures were recorded and plotted



Figure 9-Flowsheet with cooling water and heat exchanger geometry

The simulations reveal that using the as built exchanger, the excess surface in the condenser design results in lower process outlet temperatures. This difference, if left unattended, might change the LLE split in the flash tank, which, in a process this sensitive, could upset the stability of the process possibly necessitating a redesign. The sensitivity analysis does show however that if we are willing to return the cooling water at 103.7°F the design temperature of 150°F can be maintained. If this is unacceptable, some redesign of the process or the condenser would be required.

COST ANALYSIS

Using CHEMCAD's economic features we can:

- i. Estimate the equipment costs using a Guthrie type analysis;
- ii. Estimate the installed costs using a factored method;
- iii. Estimate battery limit costs by adding in miscellaneous items;
- iv. Estimate operating costs using feed and utility flows determined by the simulation;
- v. Calculate a project net present value.

INITIAL COMMENTS

The above analysis can be done very quickly from a few hours to a few days depending on the system. We now have a complete model which gives us a systematic way of;

- i. Determining where further research should be done;
- ii. Identifying and pursuing other lines of investigation;
- iii. Evaluating the economic impact of design alternatives.

By way of example, we might now pursue the following:

- i. The initial runs illustrated that the process is very sensitive to the LLE in the condenser flash drum which in turn is temperature dependent. However up to this point we have not used any LLE data at all. The LLE was predicted using VLE BIP's. Therefore, a literature search and/or lab measurements of LLE will be necessary before a final design can be achieved.
- ii. The sensitivity of this process will also generate control problems. Early investigation here will improve operability.
- iii. Our current design is at a single steady state. Clearly disturbances will need to be analyzed not only to determine economic impact, but also to examine plant operability and flexibility.
- iv. The decant water stream is going to have to be cleaned up before it can be discarded. What is the best way of doing that? Can the process be altered to produce less water or cleaner water?

DISTURBANCES IN THE ETHANOL UNIT

Let us now return to our azeotropic distillation problem to see how operability issues might impact our preliminary design.

What happens if the feed composition or flowrate changes? What if impurities get into the feed stream? What is the effect of changing cooling water temperatures? These issues can impact equipment sizes and process design. Below you will see the flowsheet and response histories to hypothetical conditions raised by all of these questions.







In the above example, the column pressure is controlled by varying the cooling water to the condenser. The pressure controller (PID) Unit No. 7 "senses" the column pressure, calculates an error function and generates a control signal for the control valve (Unit No. 6). Based on the control signal, the valve opens and closes, regulating cooling water flow to the condenser. The energy removed (or not removed) from the column determines the column pressure. This flowsheet requires only a simple modification to our last flowsheet.

Unit No. 5 of the flowsheet is a discreet event scheduler. In one simulation it was used to vary to cooling water temperature to the condenser over a range of 80-100°F. The response of the column pressure is shown in 10.

In a second simulation, the scheduler was used to introduce a small impurity (amyl alcohol) in the feed over a period of 20 minutes. The simulation then determined how long it would take the system to return to its product impurities spec about 10 ppm (on a mole basis). The impurity was started at t = 30 minutes and was gone 40 minutes later.

The simple examples are not intended, of course, to be comprehensive but illustrative. Since moving from a steady-state simulation to a dynamic one is a simple matter (and since moving from dynamics to steady-state is equally simple), many issues of operability and safety, which directly impact the process design, can be included at a very early stage where they can be addressed in the most comprehensive (read practical and economical) manner. Reworks in design and in the field can be dramatically reduced. Since the tools for this procedure are now fully integrated, errors are minimized and work flows smoothly and quickly.

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