Memo 9

DIVERSIFIED CHEMICAL PRODUCTS

Specialty Products Division
Cambridge MA

TO: U. R. Engineer
FROM: I. M. Supervisor
DATE: 2007 Sep 28
SUBJECT: Lucretex Base Case Simulation

I am requesting that you carry out a base case simulation of the entire batch process for the production of the monomers for Lucretex from given raw materials. All the process operating parameters are specified below. Specifically, you should develop complete mass and component mole balances for the entire flowsheet with the specified base case operating parameters. Once you have completed the simulation, you should document the results in *Section 4: Base Case Process Simulation* of the Final Report. Please submit Section 4 in class on 2006 Oct 5.

I am also interested in understanding the economics of the batch process design at base case conditions. As a first step, you should compute size factors for each stage in the process. For the two cases of no intermediate storage (NIS) and unlimited intermediate storage (UIS), identify the limiting unit(s). Calculate the average production rate of (A+D) for each storage policy. As mentioned in Memo #8, we need 310,000 lb of (A+D) of 99% purity by mass. Calculate the total campaign time and costs in $/lb needed to achieve this objective for both storage cases. Your cost estimate should include the cost of raw materials, waste processing, recycle credit, utilities, and equipment rental. All required economic data are provided in Memo #8. After you finish your economic analysis, please document the results in *Section 5: Base Case Economic Analysis*. Please submit Section 5 in class on 2006 Oct 16.

The base case flowsheet should be simulated according to the following recipe:

1. Reaction I

Reactor size:	500 gal
Raw materials:	460 kg R1
	540 kg R2
	5 L Pt catalyst/toluene slurry
	690 kg toluene
Molar concentration of Pt in undiluted slurry:	5 mol/Ll
Jacket heating rate:	0.0 kcal/h

<u>Operating procedure:</u>
Charge 25% of R1 and R2, and all of the toluene
Heat the charge to 60 ºC
(Use JACOBIAN to simulate from this point)
Charge all the catalyst slurry to initiate reaction
Feed the remaining reactants at a constant rate over 8 hours
Continue reaction for another 4 hours
Cool reactor contents to 65 ºC

Note: Find maximum volume required during reaction.

2. Reaction II

Reactor size:	750 gal
Raw materials:	All the materials from Reaction I
	110 kg MeOH

Operating procedure:
Charge material from Reaction I
Charge all the methanol
Temperature of reaction = 65 ºC
Stopping criterion: molar conversion of C to E = 0.98

3. Distillations I and II

Still size:	750 gal
# of theoretical stages:	8
Feed:	All the material from Reaction II
Assumptions:	Lump R1, R2, C, and I1 into R1 (add all the mole fractions)
	Lump I2, Pt, and Pt* into I2

Operating procedure:
Charge the material from Reaction II
Heat to steady state under total reflux at vapor rate: 15 kmol/h
(Use JACOBIAN to simulate from this point)
Reflux ratio: 7; constant for distillations I and II
Pressure (distillation I): 760 mm Hg
Stopping Criterion: Pot temperature reaches 135 ºC
Divert overheads to second accumulator
Begin reducing pressure from 760 to 80 mm Hg in a linear profile over 30.0 min
Continue at pressure (distillation II): 80 mm Hg
Stopping Criterion: Pot temperature reaches 135 ºC
Dispose of first cut and pot residue

Distillation Cuts:
One overhead cut from Distillation I (First cut)
One overhead cut from Distillation II (Second cut)
Pot residue from Distillation II

4. Reaction III

Reactor size:	500 gal
Raw materials:	Second cut from above distillations
	30 moles water per mole E in the cut

Operating procedure:
Charge all of the second cut

Charge all the water
Heat to reaction temperature
Temperature of reaction = 90 ºC
Stopping criterion: molar conversion of E to D = 0.88

5. Distillation III

Still size:	1250 gal
# of theoretical stages:	8
Feed:	All the material from Reaction III

Operating procedure:
Charge the material from Reaction III
Heat to steady state under total reflux at vapor rate: 15 kmol/h
(Use JACOBIAN to simulate from this point)
Reflux ratio: 6
Pressure: 760 mm Hg
Stopping Criterion: purity of (A+D) in the pot = 0.99 (mass)

Distillation Cuts:
One overhead cut
Pot residue at end of distillation