

DIVERSIFIED CHEMICAL PRODUCTS
Specialty Products Division
Cambridge MA

TO: U. R. Engineer
FROM: I. M. Subcontractor
DATE: 2006 Oct 6
SUBJECT: Lucretex Batch Process Development Project Description and Goals

Per your request I obtained the data you need for the economic analysis. Here are the results of my calculations:

- Reaction 1: The reaction time is 39,600 s, the maximal liquid volume 1.585 m³ and the maximal cooling load in the condenser 48.8 kJ/s. At the end of the reaction the volume is 1.558 m³ and the temperature 378 K.
- Reaction 2: The reaction takes 14,627 s. 3120.9 mols of methanol are needed for the reaction. The inlet volume is 1.615 m³ and the outlet volume 1.560 m³.
- Distillation 1: The simulated distillation time (from moment of first draw until temperature constraint) is 15,719 s. The distillation overhead consists of 1412.3 mols methanol, 1496.4 mols R1, 6420.2 mols toluene, 6.37 mols E and 3.67 mols A.
- Distillation 2: The simulated distillation time (from moment of vacuum initiation until temperature constraint) is 6391 s. The distillation residue (bottom) consists of 0.10 mols active catalyst, 24.90 mols deactivated catalyst, 1.005 mols I2, and 64.30 mols A.
- Reaction 3: The reaction time is 17,112 s and 51068 mols water are needed. The inlet volume is 1.659 m³ and the outlet volume 1.820 m³.
- Distillation 3: The simulated distillation time (from moment of first draw until purity constraint) is 89,301 s. The distillation overhead (top) consists of 1446.9 mols methanol, 873.7 mols toluene, 255.3 mols E, 216.4 mols A, and 50345 mols water. The pot fulfills the purity specification with 723.5 mols D, 1982.2 mols A, and 86.06 mols toluene.