Final Project Report – Team 3

TenTen Specialties
Business Development

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SUBJECT: Preliminary Design for HDA Process

Summary
Benzene is a widely used, and therefore highly demanded, chemical. It is a major part of gasoline and is used to make plastics, resins, synthetic fibers, detergents, pesticides, and more. Our goal is to design a hydrodealkylation (HDA) process that can support the production of 80,000 Mg of 99.5 wt% benzene a year. Our preliminary design proposes a plant that produces 106,415 Mg of 99.5 wt% benzene a year. Considering the annual shutdown needed for maintenance, the process operating year is 350 days of 24 hours. The fixed capital investment is $261,451,200 and the working capital investment is $10,415,300, summing to a total capital investment of $271,866,400. With an annual revenue of $160,424,100 and an annual operating cost of $119,384,100, the plant is expected to make an annual profit of $41,040,100. The payback or breakeven time is 6.6 years.

Process Overview
The 99.5 wt% benzene is produced through the HDA reaction of toluene with hydrogen.

$$H_2 + C_7H_8 \rightarrow CH_4 + C_6H_6$$

Our design utilizes a mixer, furnace, plug flow reactor (PFR), furnace, separator pot, distillation column, pump, pressure relief valve (PRV), compressor, and a flow splitter (see Figure 1). Liquid toluene is first pumped from storage and joins a fresh hydrogen stream and two recycle streams from two later operations at the mixer. The reaction occurs in vaporous form, so the combined stream of all four components are heated in the furnace before entering the PFR, where hydrogen and toluene react to form benzene and methane. The unreacted reactants and newly formed products are then cooled in the condenser and separated by phase in the separator pot. The vaporous phase of hydrogen, methane, toluene, and benzene leaving the separator are split into a purge stream, which is used as a fuel gas, and a recycle stream, which goes back to the mixer. Before entering the distillation column, the liquid stream from the separator passes through a PRV because distillation occurs at low pressure. Most of the benzene and a small amount of toluene are taken overhead from the distillation column in liquid form for storage. The stream that consists of the leftover benzene residues and most of the toluene is then pumped back to the mixer as a second recycle stream. It joins the two inlet reactant feeds and the first recycle stream and the process proceeds.

Details of Design

Our design ensures that all mass and energy balances are satisfied while meeting the operating conditions specified for safe operations. The proposed process limits toluene conversion under 50% and uses an excess of hydrogen to suppress side reactions.

The initial iteration of the plant featured a breakeven time of 8.8 years. We began altering parameters with the goal of decreasing the breakeven time (see Table 1). We first increased the toluene input, which greatly increased the amount of benzene produced and increased our profit rates by over 60%. We then altered the ratio of the distillate to the bottoms stream in the distillation to get more benzene out from the overhead (refer to Table 2 for the stream table). By lowering our fixed costs and increasing our benzene production by 31%, we improved the profitability and decrease the number of years required to break even by 2.2 years, from 8.8 years to 6.6 years. Although the total initial capital investment increased by 28%, the annual profit of the plant increased by 69%.

Mixer
Our design process revolves around twelve parameters, as seen in Table 1, that can be optimized to produce 99.5 wt% benzene. The initial molar flow rate of toluene was increased, which increased the toluene conversion. The initial molar flow rate of hydrogen, via the hydrogen to toluene ratio, was also increased to produce a greater quantity of benzene. We increased the hydrogen to toluene ratio to be greater than one to have excess hydrogen, which suppresses the undesired side reactions, such as the formation of diphenyl.

Furnace
The components of the inlet stream, when heated, are all assumed to be ideal gases, so we used Raoult's Law to calculate vapor and liquid molar flows. The outlet temperature remained fixed at 820°C to heat the liquid toluene to vapor form before entering the reactor. The pressure was decreased by 0.5 bars to 30 bars during the process. Neither the temperature nor pressure were varied during our optimization because they were at values that allowed for the reaction to occur.

Reactor
The design of the reactor assumes adiabatic conditions and no tubes and catalytic constraints. Three reactor parameters are fixed to minimize cost and maximize the productivity of the plant. For example, the inlet reactor temperature is fixed at 820°C. A higher temperature would result in a high conversion of toluene and increased equipment cost. In addition, the reactor diameter is 0.3 m to keep the velocity along the reactor under 20 m/s. Doing so ensures that the catalysts remain in the reactor and the residence time is high. Lastly, the reactor length is kept around 5 m to lower costs and limit toluene conversion.

Condenser

The outlet stream from the reactor enters the condenser, where it is cooled. The equipment and maintenance cost of the condenser depends on the heat duty and surface area of the vessel, which are affected by the condenser outlet temperature. Thus, the outlet temperature is set at 120°C. It is low enough to meet the requirements of later operations, such as the distillation column, but high enough to minimize costs.

Separator Pot

The stream leaves the condenser to the separator pot where the components are separated by their phases. The pressure of the outlet stream is fixed at 28 bar to gradually reach a low pressure, which is required for distillation.

Flow Split

The vaporous materials are sent to a split stream to be purged or recycled. The split fraction is fixed at 0.5 to reduce waste and prevent accumulation.

Compressor

The first recycle stream that consists of hydrogen and methane passes the compressor before entering the mixer. The compressor increases the pressure of the inlet stream to 30.5 bars. The decision was made so that the stream entering the reactor to have a pressure of 30 bars. The high pressure allows a high reaction rate.

Pressure Relief Valve

The liquid materials are sent to a pressure relief valve which reduces the pressure, allowing for more vapor to enter the distillation column. In our iteration, we changed the inlet pressure from 2 to 3 bars, which decreased the capital cost of distillation.

Distillation Column

One of the biggest changes that helped our process was lowering the desired benzene mole fraction (ySpec) in the distillate. ySpec was initially set at 0.96, so our benzene products were purer than the required 99.5 wt%. We find that lowering it to 0.9958 still guarantees the production of 99.5 wt% benzene while decreasing the capital cost of the reactor. Moreover, the distillate to feed ratio was increased from 0.2 to 0.4 to get more benzene product from the overhead. Lastly, the reflux factor was kept at 1.3, the typical value used in industry.

Pump

The pump is used to increase the pressure of the bottoms stream from the distillation to 30.5 bars. Please see *Compressor* for the explanation of the choice of pressure. The stream, which contains benzene and toluene, goes back to the mixer.

Figures and Tables

Figure 1: HDA Process Diagram

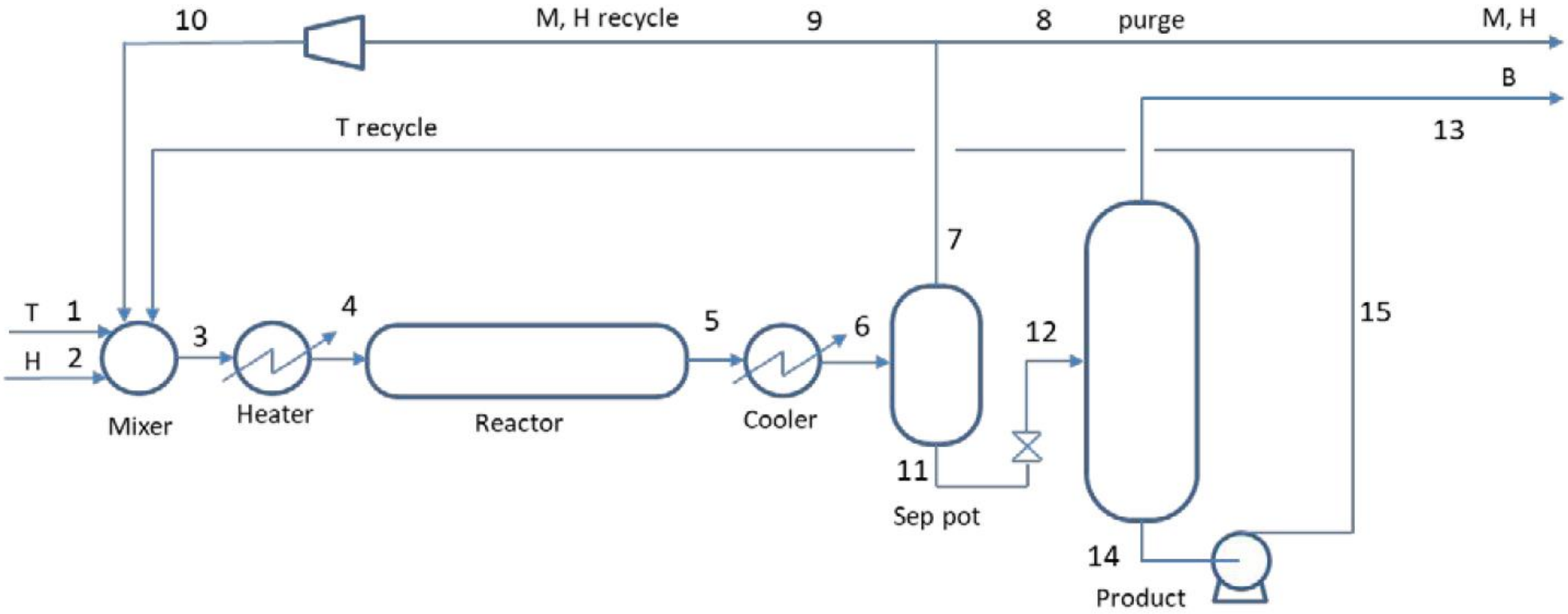

Table 1: Results of Optimization

		Initial Run	Final Run
Parameters	Inlet Reactor Temp (°C)	820	820
	Inlet Reactor Pressure (bars)	30	30
	Outlet Condenser Temp (°C)	120	120
	Outlet Sep. Pot Pressure (bars)	28	28
	Purge to Recycle Split Fraction	0.5	0.5
	Initial Toluene Feed (mol/s)	40	50
	Initial Hydrogen to Toluene Ratio	1.5	1.1
	Inlet Distillation Pressure (bars)	2	3
	Benzene to Toluene Ratio (ySpec)	0.996	0.9958
	Distillate: Feed	0.2	0.4
	Reflux Factor	1.3	1.3
	Reactor Diameter (m)	0.3	0.3
	Reactor Length (m)	5	5
Results	Toluene conversion	0.3719	0.4984
	TCI (k$)	212774	271866
	Profit (k$)	24296	41040
	BET (year)	8.8	6.6
	Benzene 99.5 wt% (Mg)	81,384	106,415

Table 2: Stream table

Stream	Liquid Toluene 1	Hydrogen 2	Mixer Outlet 3	Furnace Outlet 4	Reactor Outlet 5	Condenser Outlet 6	Vapor Products 7	Purge Stream 8	M, H Recycle 9	Compressor Output 10	Liquid Products 11	PRV Output 12	Benzene Products 13	Distillation Bottoms 14	B, T Recycle 15
Hydrogen Feed (mol/s)	0.00	55.00	61.28	61.28	12.57	12.57	12.57	6.28	6.28	6.28	0.00	0.00	0.00	0.00	0.00
Methane Feed (mol/s)	0.00	0.00	48.72	48.72	97.43	97.43	97.43	48.72	48.72	48.72	0.00	0.00	0.00	0.00	0.00
Benzene Feed (mol/s)	0.00	0.00	24.86	24.86	73.58	73.58	7.33	3.67	3.67	3.67	66.25	66.25	45.05	21.20	21.20
Toluene Feed (mol/s)	50.00	0.00	97.76	97.76	49.04	49.04	2.19	1.09	1.09	1.09	46.85	46.85	0.19	46.66	46.66
Temperature (C)	25.00	25.00	153.51	820.00	886.10	120.00	119.56	119.56	119.56	125.72	119.56	119.56	120.61	141.54	143.69
Pressure (bar)	30.50	30.50	30.50	30.00	29.96	29.46	28.00	28.00	28.00	30.50	28.00	3.00	3.00	3.00	30.50
Enthalpy (J/s)	0.00	0.00	-8.20E+05	2.31E+07	2.51E+07	-1.80E+06	4.77E+05	2.39E+05	2.39E+05	2.55E+05	-2.27E+06	-2.27E+06	-8.12E+05	-1.10E+06	-1.08E+06
Liquid Hydrogen (mol/s)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liquid Methane (mol/s)	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
Liquid Benzene (mol/s)	0.00	0.00	20.16	0.00	0.00	66.56	0.00	0.00	0.00	0.00	66.25	66.25	43.38	21.05	21.20
Liquid Toluene (mol/s)	50.00	0.00	88.28	0.00	0.00	46.95	0.00	0.00	0.00	0.00	46.85	46.85	0.19	46.52	46.66