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Heat Balance Analysis for Esterification Heat Exchanger

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Abstract— **Purified Terephthalic Acid (PTA for short) and Mono Ethylene Glycol (MEG) are the basic raw materials used for polyester manufacture. In the manufacture of textile grade polyester, these raw materials are converted to molten polymer (Polyethylene terephthalate) in continuous polymerisation (CP) units. CP-4 is one such continuous polymerisation unit, feeding polymer to manufacture Polyester staple fiber (PSF). in Maral Oversease limited, nimrani. The rated capacity of CP-4 is 180 tons per day of polymer, at present running 224TPD. Design of CP-4 unit is based on DU PONT technology.**

The paper comprises the study on CP-4 PSF esterification section heat exchanger, it discuss heat balance of the system.

Index Terms—**CP, PSF, PTA, MEG.**

I. Introduction

A heat exchanger is a device that is used to transfer thermal energy (enthalpy) between two or more fluids, between a solid surface and a fluid, or between solid particulates and a fluid, at different temperatures and in thermal contact. In heat exchangers, there are usually no external heat and work interactions. Typical applications involve heating or cooling of a fluid stream of concern and evaporation or condensation of single or multi component fluid streams. In other applications, the objective may be to recover or reject heat, or sterilize, pasteurize, fractionate, distill, concentrate, crystallize, or control a process fluid. In a few heat exchangers, the fluids exchanging heat are in direct contact. In most heat exchangers, heat transfer between fluids takes place through a separating wall or into and out of a wall in a transient manner.

In many heat exchangers, the fluids are separated by a heat transfer surface, and ideally they do not mix or leak. Such exchangers are referred to as direct transfer type, or simply recuperators. In contrast, exchangers in which there is intermittent heat exchange between the hot and cold fluids via thermal energy storage and release through the exchanger surface or matrix are referred to as indirect transfer type, or simply regenerators. Common examples of heat exchangers are shell-and tube exchangers, automobile radiators, condensers, evaporators, air preheaters, and cooling towers. If no phase change occurs in any of the fluids in the exchanger, it is sometimes referred to as a sensible heat exchanger. There could be internal thermal energy sources in the exchangers, such as in electric heaters and nuclear fuel elements.

Combustion and chemical reaction may take place within the exchanger, such as in boilers, fired heaters, and fluidized bed exchangers. Mechanical devices may be used in some exchangers such as in scraped surface exchangers, agitated vessels, and stirred tank reactors. Heat transfer in the separating wall of a recuperator generally takes place by conduction. However, in a heat pipe heat exchanger, the heat pipe not only acts as a separating wall, but also facilitates the transfer of heat by condensation, evaporation, and conduction of the working fluid inside the heat pipe. In general, if the fluids are immiscible, the separating wall may be eliminated, and the interface between the fluids replaces a heat transfer surface, as in a direct-contact heat exchanger.

II. HEAT BALANCE

The formation of DHET with the elimination of two moles of water is starting reaction of manufacturing of PET .The subsequent reaction where in two/more such DHET molecules join together to build a chain of polymer involves elimination of one molecule of MEG. This is condensation polymerization.

A both reactions are reversible and removal of byproduct namely water and MEG has to be done to drive reaction in forward direction to produce PET polymer.

The heat of reaction can be calculated using following reaction at 25 °C.

The heat of reaction of PTA and MEG = {Sum of heat of formation of products - Sum of heat of reaction of reactants}

Reactants of Formation	**Heat of Formation**	**Products**	***A. Heat of Formation***
1mole of PTAkcal/mol	-195.02 kcal/mol	1 mole of DHET	-261.80
2 mole of MEGkcal/mol	-92.07 kcal/mol	2 mole WATER	-57.79

$$= \{(-261.80) + 2(-57.79)\} - \{(-195.02) + 2(-92.97)\}$$

$$= +3.54 \text{ kcal/mol}$$

Hence standard heat of reaction at 25 °C is 3.57 kcal/mol. As the value is small and +ve, the reaction is slightly endothermic.

As the plant data shows high heavy heat load duty at the reactor stage wherein the initial reaction forming DHET

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takes place. The high heat duty can be requirement for higher production to increase the rate of reaction or to keep process fluid in molten form.

Polymerization reaction involving the chain building of monomers with elimination of MEG Is exothermic reaction. The heat of reaction given in literature is –20 kcal/mol of MEG given out. When the above values are very small, so heat of reaction is considered negligible in heat balance calculation.

III. DESIGN CALCULATIONS

Polymer Through PUT	**Flow 9330 kg/hr (Data)**
Specific heat of PTA	1.312 kJ/kg.°C
Avg. specific heat of EG	2.42 kJ/kg.°C
Heat of dissolution of PTA	472 kJ/kg.°C
Specific heat of water	4.184 kJ/kg.°C
Heat of vaporization of EG at (285°C)	573 kJ/kg.°C
Heat of vaporization of water at(285°C)	1439 kJ/kg.°C
Specific heat of oilgomer	2.09 kJ/kg.°C
PET Actual	9165.50 kg/hr
PTA feed	7892.40 kg/hr
Recycle EG feed (with 5%moisture)	6205.05 kg/hr
Actual EG	5895 kg/hr
Water	310.30 kg/hr
Water vapor overhead	1887 kg/hr
EG vapor overhead	2735 kg/hr
Slurry temp.	80 °C
Reactor temp	285 °C

HEAT CALCULATIONS

Q	**Description**	**For PUT 9330 kg/hr**
Q1	Heat taken by PTA	$2122740\ kJ/hr$
Q2	Heat taken for PTA dissolution	$3725212.8\ kJ/hr$
Q3	Heat taken by feed EG	$2924509.5\ kJ/hr$
Q4	Heat taken by water	$266150.5\ kJ/hr$
Q5	Heat taken for EG vaporization	$1567155\ kJ/hr$
Q6	Heat taken by water vaporization	$2715393\ kJ/hr$
Q7	Heat taken to heat oligomer	$891123.75\ kJ/hr$
Q	**TOTAL HEAT LOAD**	$4212284.5\ kJ/hr = 3396817.5\ kcal/hr$
	HEAT GIVEN BY DOWTHERM	$51263\ kg/hr$

IV. RESULT ANALYSIS, CONCLUSION AND RECOMMANDATION ANALYSIS

The detailed energy balance calculations for CP4 heat indicate that the operation of the heat exchanger under steady state condition is in order and the results are within the limits of measurement and calculation errors. The calculations does not account for unsteady state situations like plant upsets. For e.g. plant shutdown and start up, power or steam failure situations are not included in the calculations.

Apart from the heat duty, there are some operating constraints associated with the Heat Exchanger and vapor separator unit. Due to high temperature operation and evolution of large quantity of vapors (Ethylene glycol and water) from the reactor, there is some carryover of oligomer / monomer along with the vapors to the column. This carryover eventually gets washed off with separation column EG flow and gets collected in the EG hot well.

With the current throughput of 224 TPD, the reactor conditions are such that the carryover is very low. Presently, fortnightly cleaning of pot filters is done which maintains the solid content in the system.

V. CONCLUSION AND RECOMMENDATIONS

CP4 esterification system works under steady state operating condition. The mass and heat balance calculations show that the same heat exchanger can be utilized for operations at 280 TPD also. For conversion at higher throughput, the heat exchange calculations have been considered with high level and temperature operation. The additional heat duty due to increased slurry flow rate and higher temperature differential is being fulfilled by the same heat exchanger.

It is recommended that with the increase in throughput, the reactor carryover needs to be carefully watched and pot filter cleaning frequency should be optimized to prevent process upset due to choking. Feasibility of other equipments for higher throughput 280 TPD (water condenser, seperation column, UFPP Finisher) etc.can be studied.

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