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Research Article

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Study the Sensitivity Analysis, Economic Evaluation and Heat Integration of a Plant Producing Dimethyl Ether (DME) from Methanol by using ASPEN HYSIS Simulation

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ABSTRACT

In this work aspen HYSYS v8.8 was used to simulate production of DME. Fluid packaging used in this process is NRTL thermodynamic. The production process is threshold problem. based on sensitivity analysis the most sensitives parameter on the DME yield were methanol feed flow rate to distillation column and reactor, tray spacing, percentage recycles methanol and reactor conversion, rector conversion and waster production rate and rector conversion. Reactor conversion above 70% has not significant increase on DME. Also DME production is proportional to methanol feed flow rate. Tray spacing in distillation column and the DME production rate is increasing up to tray spacing of 0.67 and decrease steeply in DME production rate and became constant in DME production above 2. Not recommended to use above 0.67. Total capital cost and Utility cost for total plant were determined. The heat integration of different streams was carried out using heat exchanger network. There is no pinch temperature. Since it is threshold problem is occurred. Only minimum hot utility (Q c min=0 KJ/hr) and minimum hot utility (Q h min=9.296 KJ/hr) are needed to satisfy energy requirements from external source. The production process is threshold problem and the change in delta T min value has not effect on the hot and utility cost.

Keywords: Aspen hysys; Dimethyl ether; Sensitivity; Heat integration; Pinch

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INTRODUCTION

Dimethyl ether (DME) is the organic compound with the formula CH_3OCH_3, easy to C_2H_6O. The simplest ether, it is a colorless use in a variety of fuel applications. It is an isomer of ethanol. Dimethyl ether (DME) is Ether, non-toxic and non-carcinogenic. It has no C-C bonds and it has high H/C –ratio. DME has similar physical characteristic with LPG and this enables to store and deliver DME by using existing infrastructures with minor modifications. Thus, DME is considered to be substitute with LPG for cooking and heating purposes, but also as an aerosol propellant in spray cans. Also, DME is considered as an alternative to diesel fuel due to its high cetane number and it generates lower NOx emissions than the combustion of diesel. For these reasons, DME has high industrial interest. It can be produced from different kinds of sources such as natural gas, crude oil, residual oil, coal, waste products and bio-mass. Aspen Hysys is a tool that is able to predict the flow sheet output condition s based on the standard value of the production process of the DME foe different raw materials. The aim of this research paper is to extract data from process diagram, determine minimum temperature difference, study sensitivity analysis, economic evaluation using Aspen Icarus project evaluator for all equations and determine the Heat integration to develop heat exchanger network Design.

DME Production

Direct method of DME making process from synthesis gas compromises three main steps: water-gas shift reaction, methanol synthesis and methanol dehydration. Indirect method of DME occurs in two consecutive steps: Methanol synthesis and methanol dehydration to obtain DME. For methanol synthesis a previous reaction of methane or natural gas reforming is occurred. In total, three reactors are present in the process. The reaction of DME synthesis is mainly dehydration of methanol that is exothermic and reversible in Figure 1. In the current work, the rate expression has been selected from Methanol dehydration reaction [1-4].

$$2\ CH3OH \leftrightarrow DME+H2O$$

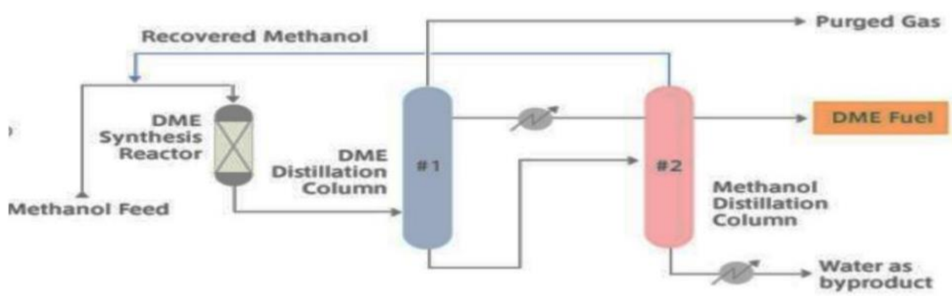


Figure 1: Overall production process flow sheet of DME

MATERIALS AND METHODS

In this work Aspen Heelys V8.8 used to simulate production of DME. Aspen HYSYS is dynamic process simulation software that is used to convert steady state process model into study time-dependent. Process simulator is defined as an engineering tool which performs automated calculations, mass and energy balances, physical property estimations, design, costing, process optimization, accurate description of physical properties of pure components and complex mixture, models for a large variety of reactors and unit operations, numerical techniques for solving large systems of algebraic and differential equations. Fluid packaging used in this process is NRTL thermodynamic. The production of DME *via* Dehydrogenation of methanol can be done using g computer aided designing and manufacturing technique to simplify tasks and to get the perfect quality and quantity product. Fresh methanol, (S1) vaporized prior to being sent to conversion reactor, operating between rates is 282.1 kmol/hr, temperature 70ºF and pressure 2 psi. A reactor condition is temperature is 400 F and Pressure is 15 psi. Assuming 80% of methanol is converted into DME in conversion reactor. Actual conversion takes place on catalytic bed reactor. Simulator Using NRTL thermodynamic model, simulate the overall process and perform sensitivity analysis. The feed methanol is then heated using heater. The reactor effluent, (S3), is then cooled prior to being sent to the first of two distillation columns. DME product is taken overhead from the first column. The second column separates water from the unreacted methanol. Reduced pressure and cold temperature were sent to the column. The methanol is recycled back to the front end of the process, while the water is sent to waste treatment to remove trace amounts of organic compounds [5-7].

RESULTS AND DISCUSSION

Regrious distillation columns were simulated using results from short cut column for first and second distillation (Figure 2).

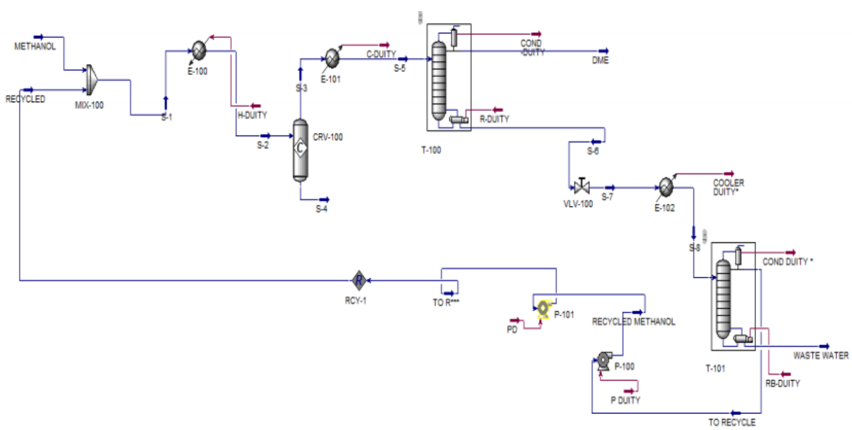


Figure 2: Over all simulated process flow sheet of DME production

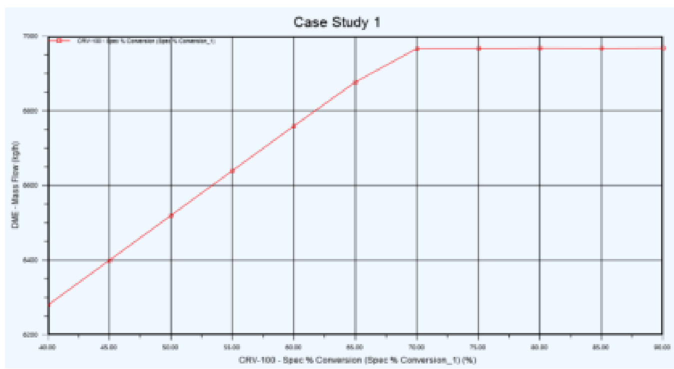


Figure 3: DME production and rector conversion

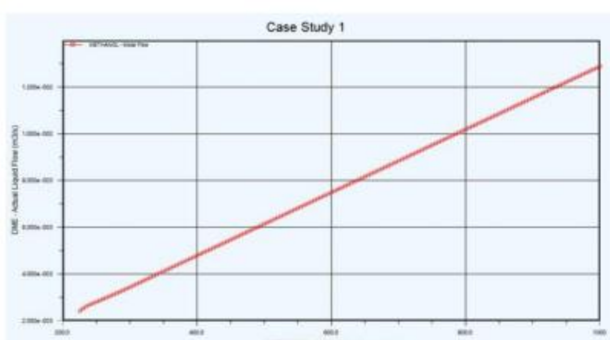


Figure 4: Feed methanol flow rate and DME actual flow rate

From Figures 3 and 4 the rate of DME production is related to the methanol flow rate and reactor conversion. Reactor conversion above 70% has not significant increase on DME. Also DME production is proportional to methanol feed flow rate.

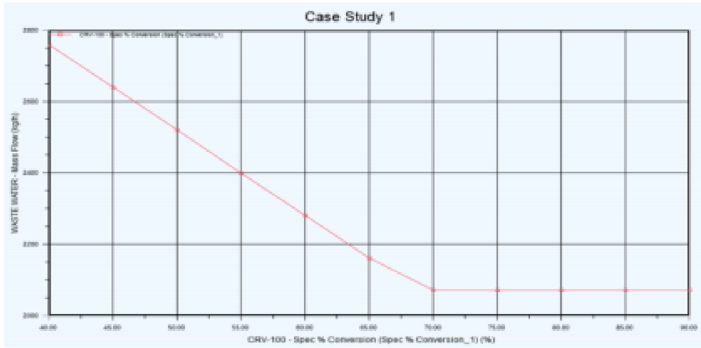


Figure 5: Rector Conversion and waster production rate

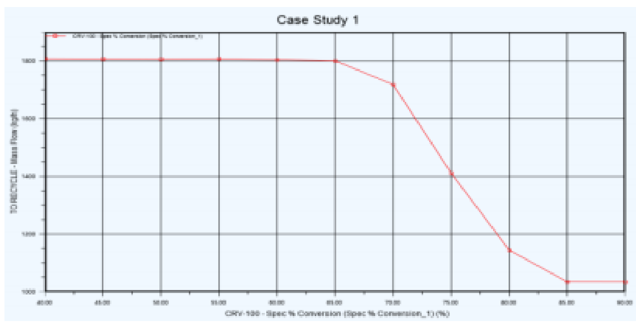


Figure 6: Percentage recycles methanol and reactor conversion

From the two Figures 5 and 6 Rector Conversion and waster production rate is related to reactor efficiency. Above 70% the rate of conversion is not significant change and water production also not much significant change. Therefor above 70% reactor conversion is not recommended. Percentage recycles methanol and reactor conversion also related by reactor performance. Rector conversions above 65%-85% the methanol recycle become decreasing up to 85%. But above this value recycle methanol will not be changed (Figure 7).

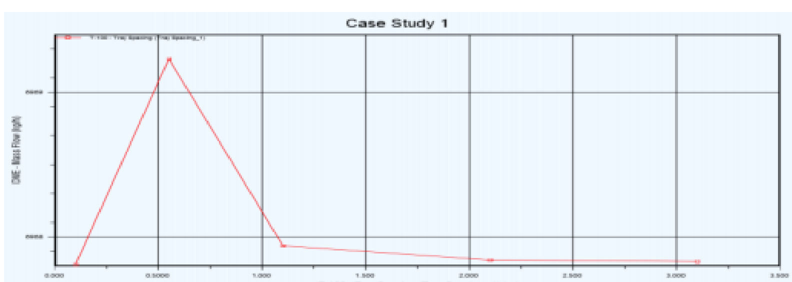


Figure 7: Distillation Tray spacing and DME

Tray spacing in distillation column and the DME production rate is increasing up to tray spacing of 0.67 and decrease steeply in DME production rate and became constant in DME production above 2. Not recommended to use above 0.67 (Figure 8).

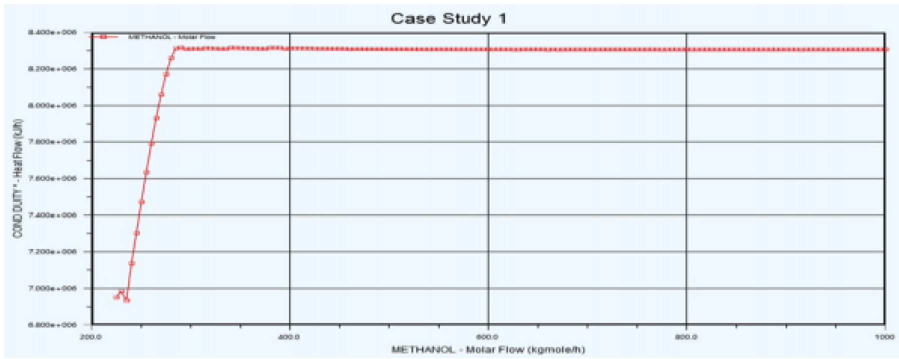


Figure 8: Methanol flow rate vs. distillation one condenser duty

Condenser duty increase as the methanol flow rate increases and became constant at flow rate of 250 kmol/kg. Increasing molar flow rate above 250 kmol/kg is resulted cost of production for pumping and heating.

Economic Evaluation

Aspen Icarus project evaluator was used for determination of total cost of production DME. Total annual operating time is 75600 hr and shelf life is 20 year. And stream price of methanol (99%) is $ 0.7-0.9/kg. And 1 kg of DME is $1.3 per kg (Tables 1 and 2).

Table 1: Total capital cost of the plan

Capital cost of the plan	
Total Capital Cost [USD]	8039470
Total Operating Cost [USD/Year]	618139000
Total Raw Materials Cost [USD/Year]	546677000
Total Product Sales [USD/Year]	790143000
Total Utilities Cost [USD/Year]	15527500
Desired Rate of Return [Percent/'Year]	20
Equipment Cost [USD]	404100
Total Installed Cost [USD	1359600

Table 2: Utility cost

Name	Fluid	Rate	Rate Units	Cost per hour	Cost units
Electricity		96.558	KW	7.483245	USD/H
Cooling Water	Water	0.180595	MMGAL/H	21.6714	USD/H

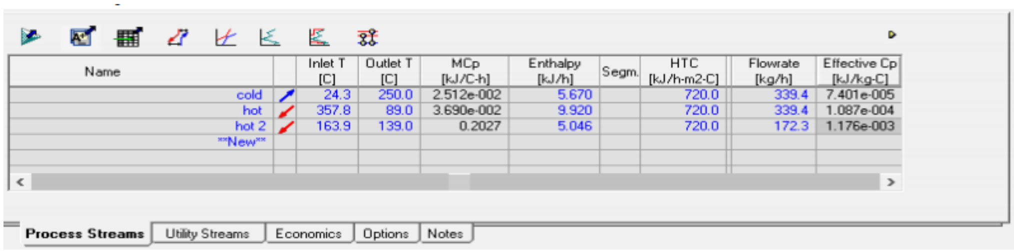
Steam @165PSI	Steam	18.05698	KLB/H	176.2361	USD/H

Heat Integration and Heat Exchanger Network Design

Data extraction of the simulated process involves the extraction of relevant stream and cost data from the process flow diagram as presented in Figures 9 and 10. The data extracted include the inlet and outlet temperatures, the heat capacities flow rate, and the specific heat capacities of all streams in the process including that of the utility streams. The following date was extracted from the PFD of the above simulated result [6] (Table 3).

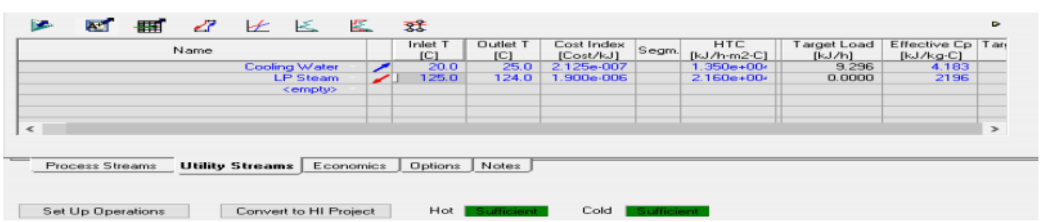
Table 3: Using newton low of thermodynamic relation the cp value was determined using heat balance. Q=m C p δ T

Location	**Stream**		**Ts**	**Tt**	**Flow rate (kmol/hr)**	**Cp J/mol.C**	**Enthalpy kJ/hr(10^6)**
E-100	Feed heater	Cold	24.27	250	339.4	74	5.67
E-101	Reactor output	hot	357.8	89	339.4	108.73	9.92
E-102	Second D. Feed	Hot	163.9	139	172.3	117.62	0.5046



Name		Inlet T [C]	Outlet T [C]	MCp [kJ/C-h]	Enthalpy [kJ/h]	Segm.	HTC [kJ/h-m2-C]	Flowrate [kg/h]	Effective Cp [kJ/kg-C]
cold		24.3	250.0	2.512e-002	5.670		720.0	339.4	7.401e-005
hot		357.8	89.0	3.690e-002	9.920		720.0	339.4	1.087e-004
hot 2		163.9	139.0	0.2027	5.046		720.0	172.3	1.176e-003
New									

Figure 9: Extracted process streams



Name		Inlet T [C]	Outlet T [C]	Cost Index [Cost/kJ]	Segm.	HTC [kJ/h-m2-C]	Target Load [kJ/h]	Effective Cp [kJ/kg-C]	Tar
Cooling Water		20.0	25.0	2.125e-007		1.350e+00	9.296	4.183	
LP Steam		125.0	124.0	1.900e-006		2.160e+00	0.0000	2196	
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Figure 10: Selected utility streams

To calculate the stream property, we can use property table and calculate the value of Cp of aqueous. In this case enthalpy is given Cp can be determined low steam and cooling water is used in utility stream which is satisfied. Assume the delta T minimum value is 10ºC (Figure 11).

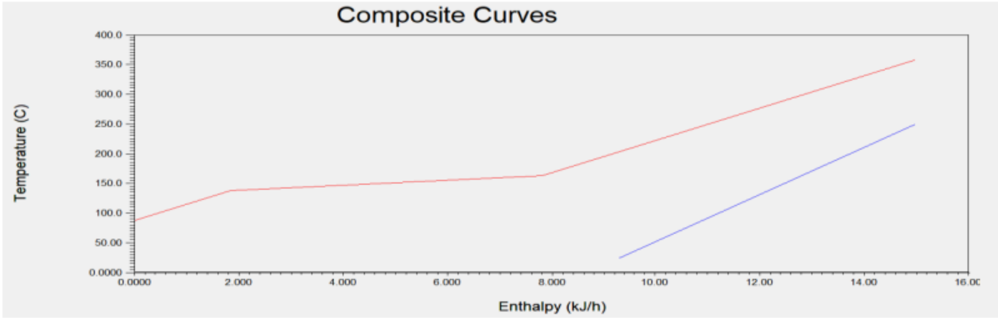


Figure 11: Composite curve

The analysis of the heat exchanger network first identifies sources of heat (termed hot streams) and sinks (termed cold streams) from the material and energy balance. Consider first a very simple problem with just one hot stream (heat source) and one cold stream (heat sink). The initial temperature (termed supply temperature), final temperature (termed target temperature) and enthalpy change (Figure 12).

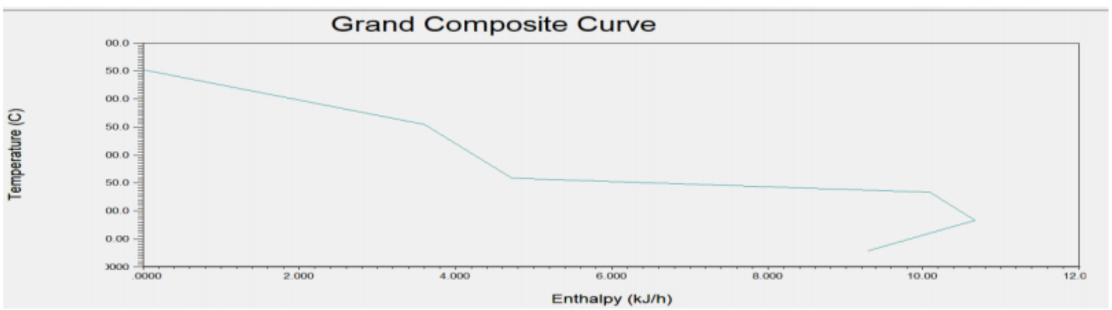
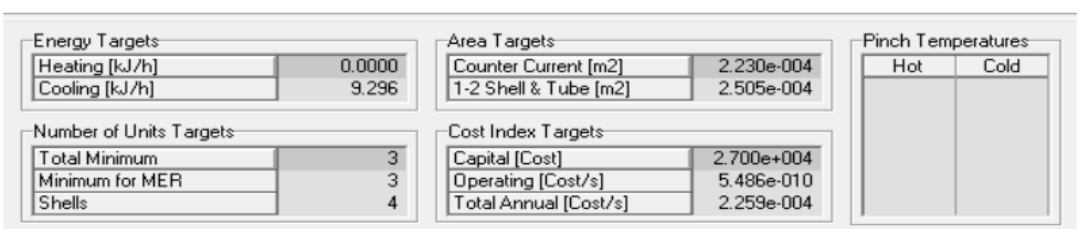


Figure 12: Grand composite curves

The grand composite curve is a more appropriate tool for understanding the interface between the process and the utility system. It shows the heat flow through the process against temperature (Figure 13). It should be noted that the temperature plotted here is shifted temperature (T∗) and not actual temperature. The grand composite curve allows alternative utility mixes to be evaluated. The profile of the grand composite curve represents residual heating and cooling demands after recovering heat within the shifted temperature intervals in the problem table algorithm [8].



Energy Targets

Heating [kJ/h]	0.0000
Cooling [kJ/h]	9.296

Number of Units Targets

Total Minimum	3
Minimum for MER	3
Shells	4

Area Targets

Counter Current [m2]	2.230e-004
1-2 Shell & Tube [m2]	2.505e-004

Cost Index Targets

Capital [Cost]	2.700e+004
Operating [Cost/s]	5.486e-010
Total Annual [Cost/s]	2.259e-004

Pinch Temperatures

Hot	Cold

Figure 13: Energy targets and pinch temperature

Heat is received from hot utility and no heat is rejected. The process acts as a heat sink. Below the pinch (in temperature terms), the process is in heat balance with the minimum cold utility, QC min. No heat is received but heat is rejected to cold utility (Figures 14-16). The process acts as a heat source. From this result it is observed that the minimum energy targets are Q c min=0 KJ/hr and Q h min=9.296 KJ/hr. there is no pinch point and called threshold problem [4].

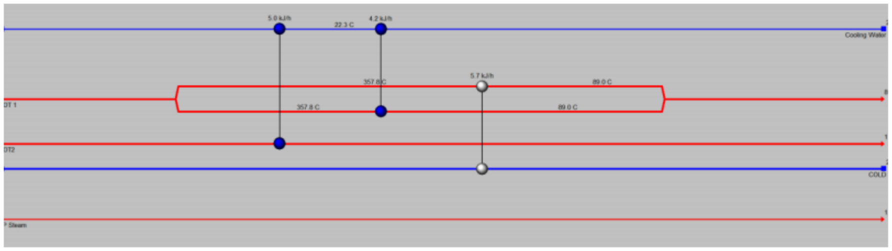


Figure 14: Heat exchanger network using HYSYS

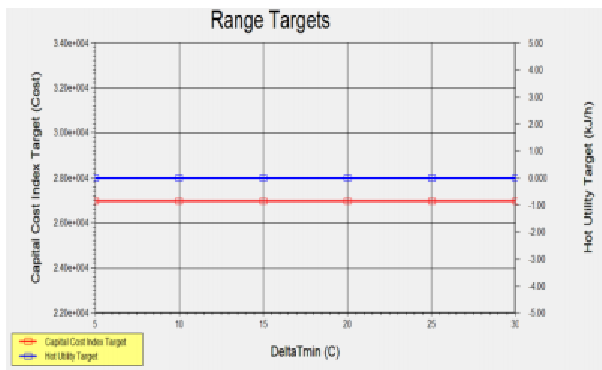


Figure 15: Effect of delta T min on capital cost and utility targets (hot utility)

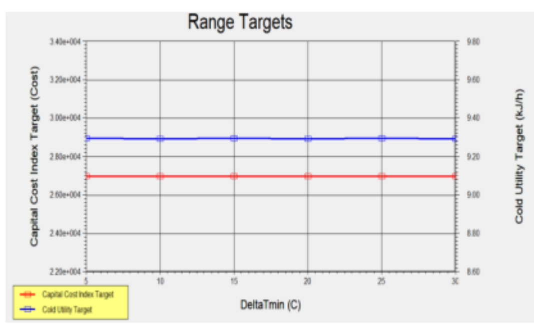


Figure 16: Effect of delta T min on capital cost and utility targets (cold utility)

The typical values of delta T minimum value are from 5°C to 30°C. The value 10°C is chosen for this problem, noting that different results will be obtained by using different temperature approaches. The problem is threshold and no cold utility needed. The effect of using different minimum approach temperatures on the economics of the process is constant. As the minimum approach temperature increases, the heat transfer area for the process heat exchangers decreases, but the loads on the hot and cold utilities increase [7]. Therefore, Effect of delta T min on investment decreases but the operating costs increase. Methods for estimating the total surface area of the exchanger network and the equivalent annual operating cost of the network are discussed in a later section. But in this project the threshold problem is occurred and the change in delta T min value has not affect on the utility and cost [8,9].

CONCLUSION

In this work Aspen Hysys V8.8 was used to simulate production of DME. Fluid packaging used in this process is NRTL thermodynamic. The production process is treshold problem. Since no pinch point was found. The production of Heat is received from hot utility and no heat is rejected. The process acts as a heat sink. Below the pinch (in temperature terms), the process is in heat balance with the minimum cold utility, QC min. No heat is received but heat is rejected. From this result it is observed that the minimum energy targets are Q c min=0 KJ/hr and Q h min=9.296 KJ/hr. This show the process is threshold and no cold utility needed and the heat exchanger is not affected by delta Tmin value. The pinch temperature of the process flow stream was threshold problem. The optimum product of DME was found 167.1 kmol/kg. NRTL is chosen as the property method in the simulation and assuming that 80% of the methanol is converted into DME in the reactor, the product stream from the reactor consists of 35% DME, 48% water and 17.8% unconverted methanol. After passing here, the separation into DME and water-methanol takes place. The converted methanol is recycled in the reactor by mixing with fresh methanol stream. Design specifications are used to meet the required results.

ACKNOWLEDGEMENT

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