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Simolation of Methyl Ethyl Ketone Production by Dehydrogenation of 2-Butanol

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Abstract: ***This paper aims to design a factory model for the production of Methyl Ethyl Ketone by dehydrogenation of 2- Butanol. Super pro software (version 10) was used for design. The stages of modeling and data of production lines and devices were explained and compared to manual calculations. This paper also covered the physical and chemical properties of Methyl Ethyl Ketone and its uses and other methods of producing it. The most important result of this research is the success of the modeling process and the absence between it and the data of manual accounts 0.001 and 0.0012 in the final production stages which confirms the accuracy of the program. Therefore, we recommend its use in the feasibility study of the establishment of chemical plants. The temperature concentration and enthalpy of different production stages were also studied.***

Keywords: MEK, Dehydrogenation, 2- Butanol

1. Introduction

To description the method of production of Methyl Ethyl Ketone by dehydrogenation from di butyl alcohol to be an experimental plant to high light any defects in the theoretical design. Whether these defects are in equipment or operating standards to increasing production of Methyl Ethyl Ketone. Based on the aqueous carbon group(R-R') attached to the carbonyl group, a Ketone is classified as an asymmetric or imbalanced fat Ketone with a molecular structure (CH_3-COC_2-H_5)Methyl Ethyl Ketone has several names , the most famous of which is MEK.Its most important uses are in plastics and petrochemicals, as a cleaning agent , and in the manufacture of glass fibers and plastics , as a welding agent , magnetic tapes , printing inks , solvent extraction and coating furniture and cars. Using biomass fermentation molasses by organism converts glucose into Meth acrylic acid (MAA) and (MEK)

$$C_6H_{12}O_6+H_2O+E.coli \rightarrow C_4H_8O+C_4H_6O_2+MASH \quad (1)$$

In a process known as enzymatic transformation which is a process of fermentation by a live bacteria called (saccharomyces cerevisiae and pichia pastoris) used strain (E. coli BL21). Liquid mixture will have different properties of the boiling point so distillation processes depend on the vapor properties of the liquid, pressure, mixtures. The vapor pressure of the liquid at the equilibrium pressure of the liquid at the equilibrium. Pressure exerted by the molecules that leave and enter the surface of liquid.

2. Materials and Methods

2.1 Description of Process

2-Butanol is dehydrogenated to produce methyl ethyl ketone according to the following equation

$C_4H_{10}O \rightarrow C_4H_8O + H_2$ (2)

2-butanol MEK hydrogen

The preheated vapors secondary butyl alcohol is passed through a reactor containing a catalytic layer of zinc or usually copper oxide which helps to Dehydrogenate the secondary 2-butanol alcohol at normal atmospheric pressure to convert it from secondary butyl alcohol to MEK .This process done in stoich –reaction from them the temperature of the gases emitted from the reactor (i.e. the product gases MEK)is raised most of the unreacted gases and alcohol are heated in pre parathion 84 -92% of alcohol and hydrogen .Purification stage which produces 99.9% of pure MEK product from the product leaving the heater the temperature in this unit is usually 79.6°C and may increase the liquid mixture will have different properties of the boiling point so distillation processes depend on the vapor pressure properties of the liquid mixtures .The vapor pressure of the liquid at the equilibrium pressure of the liquid at the equilibrium pressure exerted by the molecules that leave and enter the surface of liquid .

The first step is to list all the reactants components and catalysts involved in the production process (2-butanol - hydrogen -MEK) + (nitrogen -oxygen -water as constant). The materials used in the process are2-butanol methyl ethyl ketone and hydrogen which are among the pre -registered substances in the super pro program on which we are making an inclusion.

Second step it is the addition of the required devices and equipment in the program the first device is usually the reactors and products are determined the reaction equation was determined and the basis of the weight of the weight of the equation is determined if it is mass or mole. Then the incoming and out production lines are included with all their information quantities temperature pressure ……..etc.

The 2-butanol enters the reactor via the line stream 1 the task of the reactor is to convert 2-butanol into MEK by dehydrogenation which escalates through the line stream 2 and the product MEK sent to heating device pre-production for entering the distillation column stream 3.

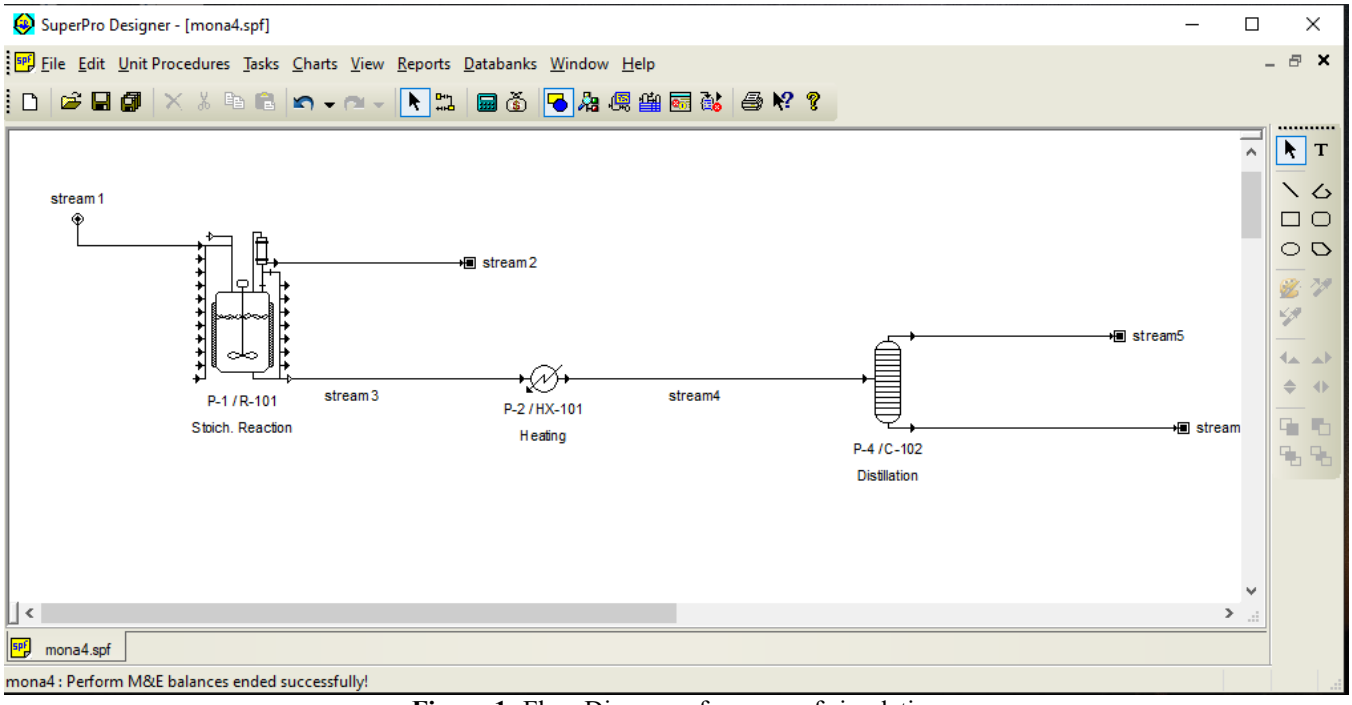

Figure 1: Flow Diagram of process of simulation

3. Results

3.1 Compering between hand calculation and simulation result

Table 1: Compares between the hand calculation and simulation results

Reactor- an arrangement	Hand calculation Kg/hr	Simulation result Kg/hr	Err (sim-hand)
Stream 1 2-Butanol	1171.8523	1171.85300	0.0007
Stream 2	H2=31.23386	H2=31.23466	0.0007
Stream 3	But=23.43649 MEK=1117.8068	But=23.43706 MEK=1117.18128	0.0006
Stream 4= stream 3	But=23.43649 MEK=1117.8068	But=23.43706 MEK=1117.18128	0.0006
Stream 5	But=0.00369 MEK=1116.95685	But=0.00469 MEK=111695785	0.001
Stream 6	But= 23.43117 MEK=0.22224	But=23.43237 MEK=0.22344	0.0012

3.2 Change of temperature during the stage

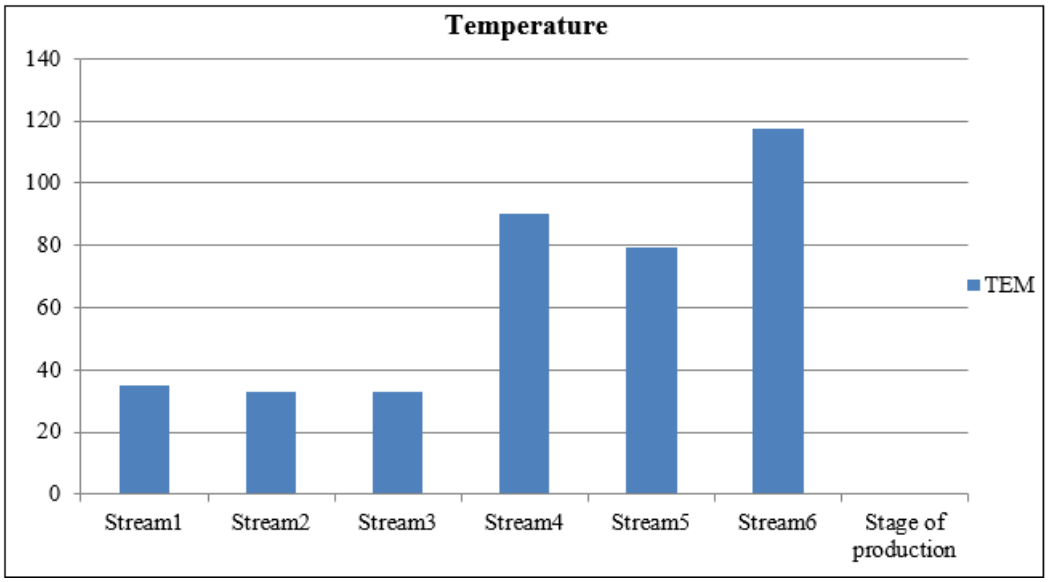

Figure 2: Temperatures along the production process

3.3 Concentration of MEK and 2-butanol during production stages

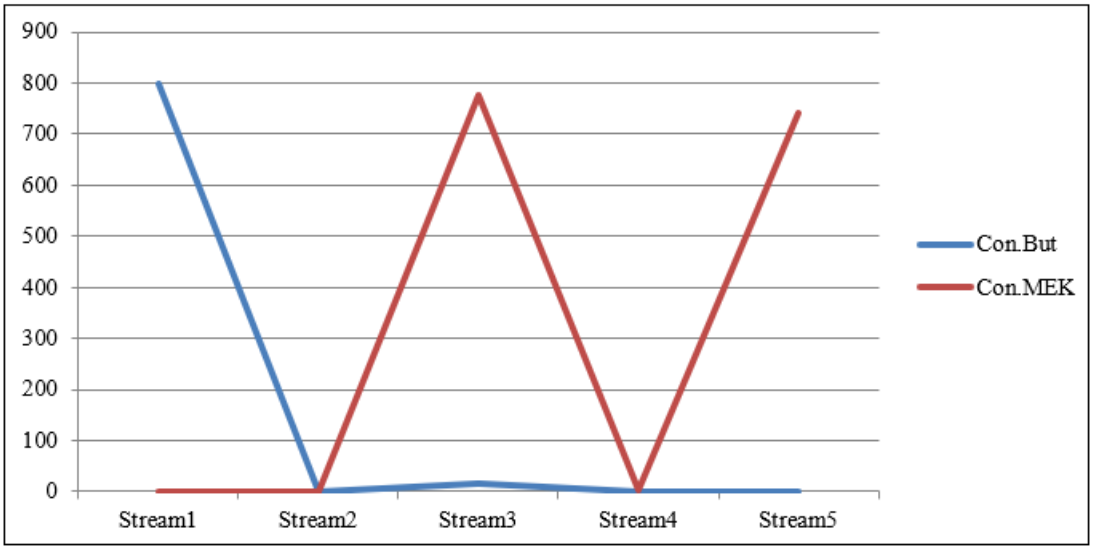

Figure 3: The concentration of reaction and produced

3.4 The changing of the enthalpy

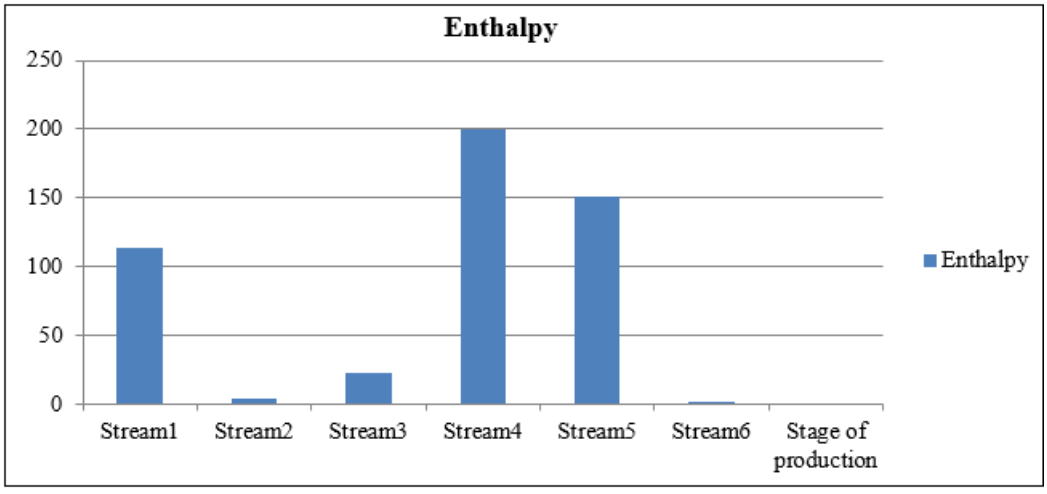

Figure 4: Changing of enthalpy

3.5 The change of specific enthalpy

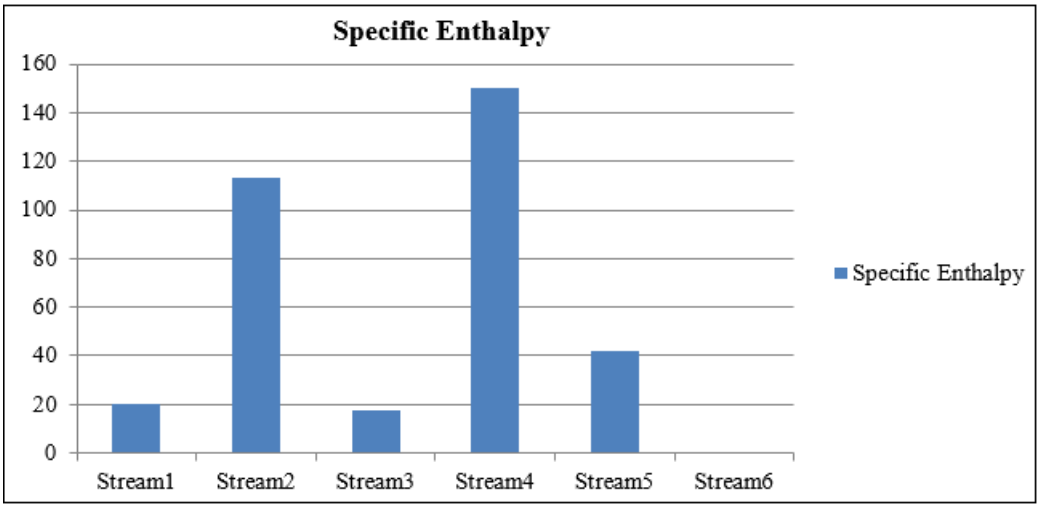

Figure 5: The Specific enthalpy

3.6 Changing of the Specific heat

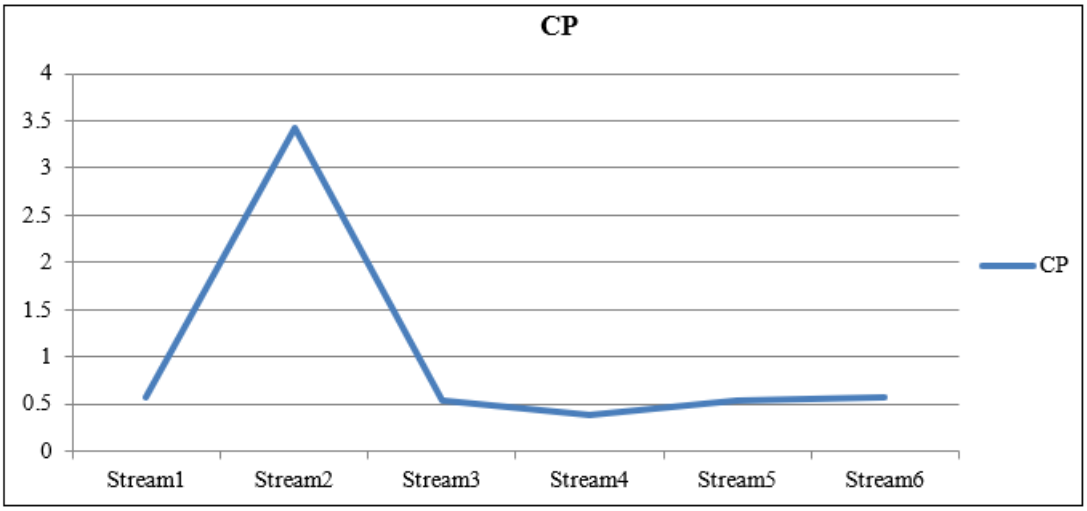

Figure 6: The Specific heat during MEK

4. Discussions

Compering between hand calculation and simulation result

Figure (1) shows the hand calculation of the material balance and the simulation result of material balance and the different between them and can be clear that there are no big different between the two result and the result of the simulation calculation is better than hand calculation

Change of temperature during the stage

Figure number (2) shows the increase of the temperature with the production stages due to the exothermic reaction of dehydrogenation of 2-butanol to methyl ethyl ketone

Concentration of MEK and 2-butanol during production stages

Figure (3) shows the increases of the concentration of the produced material (MEK) and decreases of the concentration of the reactant (2-butanol)

The changing of enthalpy

Figures (4) and (5) shows that the enthalpy and specific enthalpy was change randomly from one steps to another. Figure (5) show that drop of the specific heat during MEK production that can be measuring calories with the transfer of heat during a chemical or physical change.

4.1 Conclusion

The dehydrogenation of 2-butanol product Methyl ethyl ketone was simulated using super pro designer version 10 and it gives good result compared with the numerical calculation. The most important results obtained the production process efficiency of Methyl ethyl ketone was 99.99%. The production process takes place at a normal atmospheric pressure and temperatures between 30 °C and 120 °C. The uses of the super pro program are calculation of the cost of production equipment and materials are renewed annually and automatically without the need to recalculate the cost annually.

4.2 Recommendations

1) Use super pro designer program to develop chemical process will be very helpful because it is very accurate and useful especially in equipment design and selection of the optimum operating conditions
2) Give super pro designer more attention as importance program in academic education in universities
3) To control the economical factor and calculate income and outcome.
4) Use super pro designer in economic feasibility studies for the establishment of chemical plants

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