UNCERTAINTY IN PROCESS DESIGN AND PROCESS ECONOMICS USING HYSYS

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In process economics, equipment cost is an important element. Equipment cost is based on the size of equipment, which depends on how much process fluid is required to be treated by the equipment. HYSYS software is widely used as a simulator to design the equipments in a process industry. In order to perform simulation in HYSYS, a thermodynamic model is chosen as a Fluid package in HYSYS. This paper focuses on equipment sizing by using two different thermodynamic models and shows that for the same material and energy requirements of process fluids, there is a wide difference in sizing results of the same equipment. Further, the economic study also shows that there is a huge difference of costs for same equipment, if two different thermodynamic models are used for sizing purposes in HYSYS. The study recommends the selection of appropriate and suitable thermodynamic model to perform process designing using HYSYS.

Key words: *HYSYS, simulation, process, design, economics, thermodynamic model, cost estimation.*

1. INTRODUCTION

Chemical process plants are the combination of unit operations (phenomena involving physical changes) and unit processes (phenomenainvolving chemical changes). One of the important economical aspects of chemical plants is the amount of material and energy required to produce a product. In order to simulate the material and energy balances, the ASPEN HYSYS simulator, owned by ASPEN TECHNOLOGY [1], is widely used by academia, researchers and industrial design engineers.

For trustworthy results, the selection of appropriate and suitable thermodynamic model in a HYSYS simulation environment is very important. The need for a reliable thermodynamic model is essential when the components are not built-in in the library of HYSYS and are defined by the user. Process economics is based on the size of equipment required, which alternatively is based on the material and energy required to produce the final product. In a simulation environment like HYSYS, the requirement of the material and energy is based on the therm odynamic model or Fluid package selected in order to perform calculations. This paper is exploring the importance of selecting an appropriate thermodynamic model for simulation purposes in HYSYS and shows how a thermodynam ic model affects the whole process economics. The paper emphasizes the selections of a suitable thermodynamic model by using a case study on process equipment.

2. METHODOLOGY

Biodiesel is an alternate energy fuel, which, on industrial scale, is produced by the reaction of oil with methanol in the presence of sodium hydroxide (NaOH). The results of this reaction, callation transesterification,are biodiesel, and glycerol and soap as by-products. The production of soap is dependent on interpretive reactions conditions and could be avoided. The oil used in the current study is Jatropha oil, oil belonging to the class of non-edible oil. The Process Flow Diagram (PFD) for producing biodiesel consists of a number of equipments. One of the main equipments is the reactor where the main reaction of oil and methanol takes place. The reactor type used is Continuous Stirred Tank Reactor abbreviated as C.S.T .R. This study performs the simulations on C.S.T .R and based on the reactor sizes, the economic analysis is also performed.

There are six components involved in the reactor namely oil, methanol, sodium hydroxide, soap, biodiesel and glycerol. To perform the simulation in HYSYS, the physical and chemical properties of methanol, sodium hydroxide and glycerol were recalled from HYSY S library. Other components like soap, biodiesel and oil were defined in HYSYS using the combinations of their molecular weighs and either liquid density or boiling points. To analyze the effect of choosing different thermodynamic models on sizing results, two different thermodynamic models/fluid packages were chosen. The first was 'General NRTL' and the other was 'Glycol Package'.

Assumptions

The following assumptions were made to perform the studies;

1) The input quantities of oil, methanol and sodium hydroxide were fixed in both fluid package simulations.

2) The biodiesel in output stream from the reactor, named mixture, should have a composition of 54%.

3) Since the reactor is provided with adequate reaction conditions, there is no soap formation in the reaction products.

4) The reaction is 95% completed which means there would be some reactants present in the 'mixture' stream.

The reactor streams are shown in **Figure 1**.

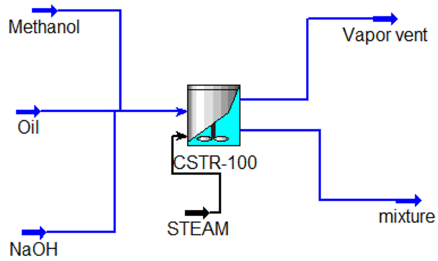

Fig. 1 Continuous Stirred Tank Reactor (C.S.T.R) – A case study

The methodology was exten ded to the whole production system shown in Figure 2 as a block diagram.The different equipments considered in the study were falling film evaporator, mixer reactor, two flash evaporators, settling tank, splitter and liquid-liquid extraction unit.

3. RESULTS

The simulation of C.S.T.R using the General NRTL thermodynamic model showed that the volume of reactor required for biodiesel production is 8.30 m3 and should have dimensions 1.917m x 2.876m (D x H). The use of the Glycol Package thermodynamic model showed that the volume of reactor required is 11.10m3 and with the dimensions of 2.112m x 3.168m (D x H).

Apparently, there should not be any such difference between the volume requirements of the reactor since both the input quantities and output composition of biodiesel are fixed. However, there is a difference in the reactor volumes triggered by the use of two dif ferent thermodynamic models. Moreover , Table 1 shows the compositions in the mixture stream calculated by two different fluid packages and highlights that there is no difference between the compositions of output stream calculated by either thermodynamic model.

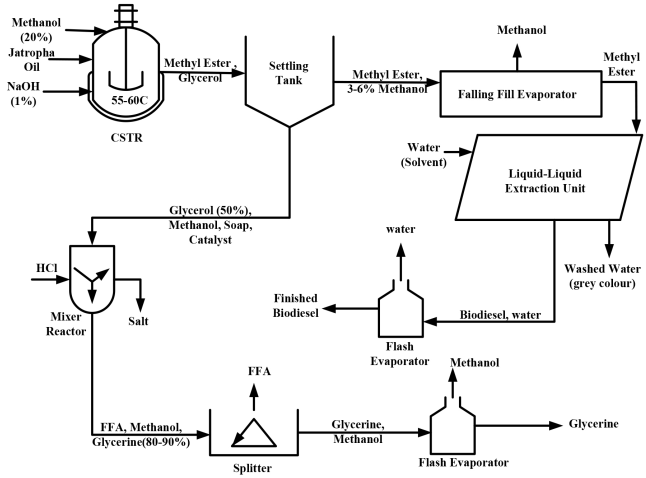

Fig. 2. Block Diagram to produce Biodiesel

Table no. 1. Compositions in output stream 'mixture'

Component	Mole Fractions (General NRTL)	Mole Fractions (Glycol Package)
NaOH	0.0644	0.0642
Methanol	0.1402	0.1400
Glycerol	0.2088	0.2088
Biodiesel	0.5400	0.5400
Soap	0.0000	0.0000
Oil	0.0468	0.0467

Process Economics

Chemical plant cost consists of two elements: one is total investment required for the project and the other is the annual operating cost [2]. Total project investment is the sum of working capital and fixed capital and the annual operating cost is the sum of variable cost and fixed cost. According to Factorial method of cost estimation, the fixed capital cost is based on the purchase costs of major equipments (PCE). Hence, knowing the purchase costs of major equipments involved in PFD, the fixed capital cost can be calculated based on those equipments. Since we assume the input quantities in both cases are the same, then the operational costs would be the same. However, there will be a difference in fixed capital cost as the reactor sizes are different.

The cost of reactor was estimated using literature [3]. The reference had cost data back to year 1967. The cost data was updated to year 2013 using the cost index of year 1967 and cost index of year 2013 (not 2014, since the cost index for year 2014 is yet to be published [4]. Cost in current year A in relation to any previous year B is calculated as [2]

Cost in year A = cost in year B $*(I_A/I_B)$

Where,

I_A/I_B = cost index year A/cost index year B

Since there was no direct cost index available from 1967 to present, the above equation was split up into two different periods: 1967 to 1980 and 1980 to 2013, respectively, as the cost index was available for these years in the literature [5][6]. Purchased costs of equipments were adopted from the literature [3] and the cost data updated to year 2013 provided the following results.

For a capacity of 8.30 m3, the reactor cost was US $90,092 and for a capacity of 11.10 m3, the reactor cost was US $120,484. This shows that there is a difference of US $30,392 between the two reactor sizes. This difference is raised just because of selection of thermodynamic model in the study. It should be mentioned here that this difference in cost is just for one piece of equipment, namely the reactor. The simulation, using two different thermodynamic models, was performed on all equipments present in the block diagram presented in Fig. 2 and sizing results were obtained. The economic analysis was performed on equipments' sizing results. Table 2 presents the costs of such equipments, using two different thermodynamic models.

Table no.2. Total cost of Major Equipments

Equipment	Cost (US $) using General NRTL	Cost (US $) using Glycol Package
Reactor	90,174	120,484
Falling Film Evaporator	75,889	101,397
Mixer Reactor	46,872	62,628
Flash Evaporator	84,817	113,327
Flash Evaporator	55,801	74,557
Settling Tank	8,928	11,929
Splitter	8,035	10,736
Liquid-Liquid Extraction	30,802	41,155
Total Cost	401,321	536,215

4. CONCLUSIONS

The process economics of a Chemical plant are based on the number and sizes of equipments required for producing a particular product. HYSYS is a simulation tool, which is widely used for sizing equipments. One of the basic steps in building a simulation environment in HYSYS, after defining components, is the selection of an appropriate thermodynamic model/ Fluid package. The current study provides an insight into the importance of selecting a reliable thermodynamic model in HYSYS. The study reveals that, having the same amounts of input and output material and energy streams, two different thermodynamic models, in HYSYS give two different capacities of a reactor. The study also shows that this difference in capacities leads to different cost estimation results, which affects the process economics. The process economics performed on a whole biodiesel production system showed that, using the sizing results of two different thermodynamic models in HYSYS, a difference of US $134,894 in total purchase costs of major equipments is observed. Total production cost is based on purchase costs of major equipments and as there is a huge difference in costs, the total production cost may be either over-estimated or under-estimated. Therefore, the current study recommends following the general guidelines in selecting an appropriate and suitable thermodynamic model/Fluid package in HYSYS, before the simulation is performed in HYSYS.

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