CAREER EPISODE 3

CE 3.1 Introduction

I shall discuss in detail the tasks that I completed for an academic project that I submitted as my final year project named as “43 kW Automobile Ethanol Reformer Design for On Board Hydrogen Production”. It was a mandatory requirement to fulfil for the completion of my bachelor degree in the Chemical Engineering from [redacted]. I was located in my university campus during the course of this project. I began working on this project on ______ and submitted my final report on _____ which made up to ____ months of total time to complete the said work.

CE 3.2 Background

CE 3.2.1

Taking practical steps towards a climate friendly world has always been my source of motivation as well as bringing innovation to help build a better and safer world. Due to the depletion of fossil fuels the world is switching towards alternative fuel sources such as hydrogen. The main concern with hydrogen fuel is its high flammability. An efficient reformer-based system is proposed for the production of hydrogen through on board reforming of ethanol to overcome the safety issues regarding the use of hydrogen safely. The hydrogen produced from ethanol reforming is further sent to the fuel cell after separation from water and other gases. The hydrogen in fuel cell reacts with the oxygen and generates power. This power can be further used to drive the motor which eventually runs the cars.

CE 3.2.2

As we all live in a world and the fossil fuel reserves are not enough for a lifelong supply for human consumption, they will vanish and the humanity has to eventually move towards alternate fuel sources. According to a research by Sustainable Minds, today the world consumes 85.2 million barrels of oil per day and this amount is expected to increase by 60 percent. According to Ecotrocity, a US survey organization, we will run out of oil in nearly 2052 and that is alarming. The environmental impact of the automobiles running on internal combustion engines happens to be very harsh. These vehicles emit poisonous gases which go into the atmosphere and their amount is increasing day by day which is causing breathing problems in infants and adults. Also internal combustion also produce a lot of noise which is resulting in the increase in noise pollution. This decreases the productivity to a drastic level and the man is not able to work properly under stress and anxiety. This project was aimed at dealing with these problems by providing a practical and modern solution.

CE 3.2.3

I fulfilled the following aims and objectives during the course of this project:

- To complete the market analysis in order to justify the feasibility of the project
- To evaluate the different processes and selected the most appropriate process
- To develop process flow diagram
- To complete the material and energy balance
- To design the required equipment
- To simulate the designed equipment for the purpose of software based analysis
- To establish the process control
- To carry out HAZOP analysis
- To complete cost analysis

CE 3.2.4

This project had an increased level of responsibility as it was an individual project which had to be completed under the supervision of the project supervisor. The following figure expresses the hierarchy that was followed for reporting during this project:

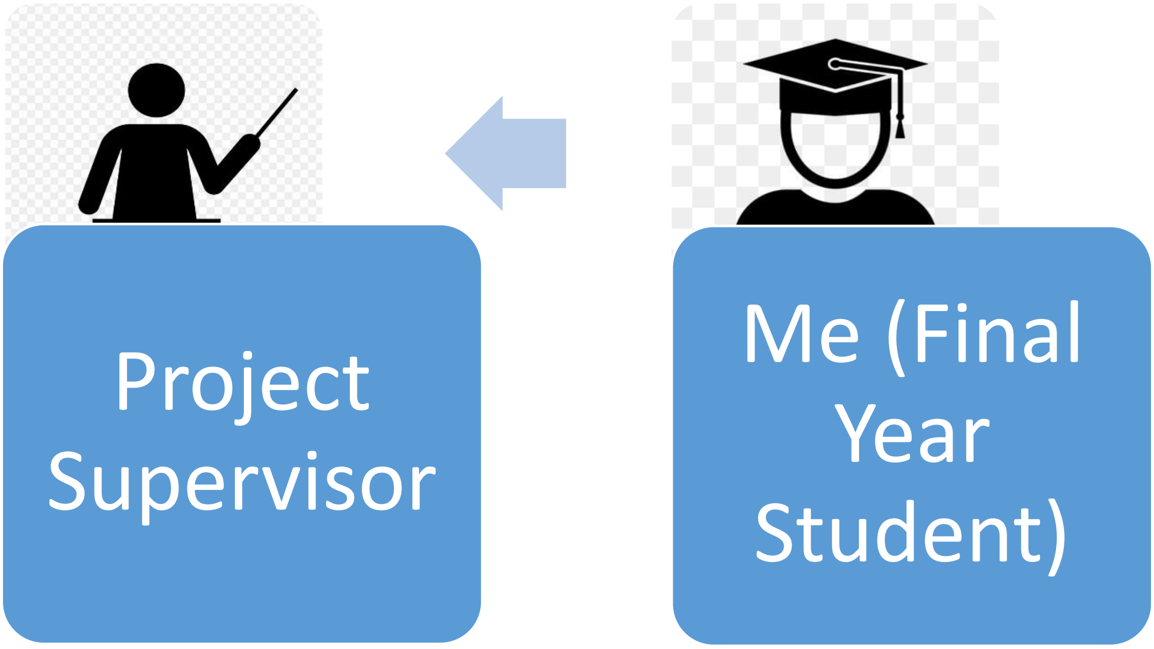

Fig. 3.1. Hierarchy for progress reporting

CE 3.3 Personal Engineering Activity

CE 3.3.1

As for the initial step of the project, I carried out a detailed market analysis in order to justify the viability of the project that I had undertaken. I observed that due to increase in global pollution and negative impact of internal combustion engine, there is an increase in the demand of hybrid and fuel cell based locomotives. Most of the major automobile industries have already shifted from ICE to alternate processes. While the rest of them are emphasizing to shift in near future. As for the market in Pakistan, I found out that the automobile market curve is flat in other countries whereas it is still rising in Pakistan and people are still moving towards buying more and more automobiles. As per the future of automobile industry, according to the above observations, lay in shifting to renewable fuel sources. I reported that most of the major automobile industries have already shifted to the alternate fuel and European Union has also given an ultimatum to the automobile makers to majorly cut the emissions by [redacted].

CE 3.3.2

I selected the process of on board hydrogen production based on biomass for powering vehicles. The depleting fossil fuels, economic constraints, high safety standards and environmental regulations have drawn the consumer attention towards the greening of automotive transportation that altogether transformed the automobile industry. Steam reforming is most common and energy-efficient process of hydrogen production which I selected for production of hydrogen. I selected this because it has high operational efficiency with low operational and production cost. The most frequently used raw materials are natural gas and lighter hydrocarbons, ethanol, and other oxygenated hydrocarbons.

The whole process comprises two stages. In the first stage, the hydrocarbon raw material is mixed with steam and fed in a tubular catalytic reactor. During this process, syngas is produced with lower content in CO_2. In the second stage, the cooled product gas is fed into the CO catalytic converter, where carbon monoxide will be converted to a large extent by means of steam into carbon dioxide and hydrogen.

CE 3.3.3

In the next step of the project I completed the process flow diagram shown below. As per the methodology I devised for this project, firstly, ethanol water mixture will be pumped where pressure of mixture is increased from 1-7 bar. The pressurized feed was then passed through a series of heat exchangers to achieve temperature of 500C desired temperature for ethanol reformer. The product gases from ethanol reformer will be further heated to 800C which was observed by me to be desired temperature of methane reformer. The product from methane reformer will be fed to the water gas shift reactor where water gas shift reaction will take place. The resulting gases from water gas shift reaction will then cooled to 60 ^oC. In the separator, water will be separated from gases. The gases will then be introduced in fuel cell where hydrogen reacts with oxygen to generate power.

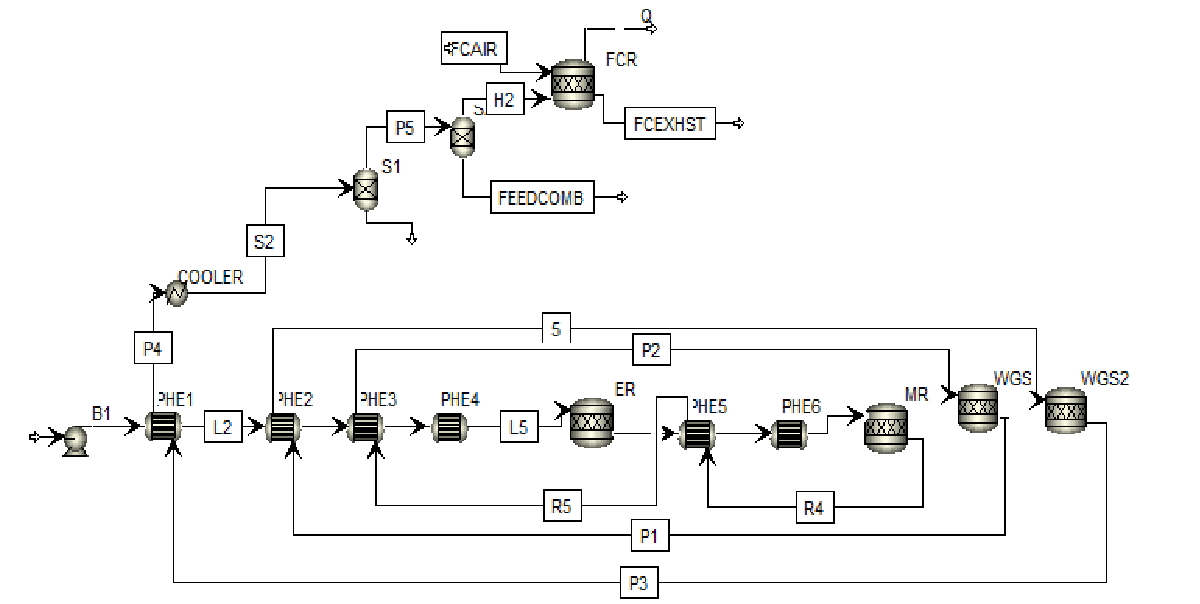

Fig. 3.2. Process Flow Diagram

CE 3.3.4

I carried out the major phase of carrying out a material balance as it helped the project to improve efficiency, maintain production, reduce environmental discharges and to maintain process control in plant. The balanced chemical equation which was used by me is as following**:**

$C_2H_5OH + 3H_2O = 2CO_2 + 6H_2O$

The basis for these are F = 750gmole/hr = 16492gm/hr whereas overall material balance was calculated by using the following formula**:**

Feed = Water+ Product (dry basis)

F = W+P

The calculations which I completed for component balance are as following:

C-Balance**:** 2*750*0.142 = 0.22P + 0.03P + 0.04P

P = (2*750*0.142)/ (0.22+0.03+0.04)

P = 734.4827586 gmole/hr = 9470gm/hr

H-Balance: (6*0.142*750) + (2*0.858*750) = (W*2) + (P*2*0.7) + (P*0.04*4)

W = 390.1034483 gmole/hr = 7021.98 gm/hr

Material balance was done by me on dry basis but the final answers shown in table are on wet basis, which was prepared by me using MS Word.

Stream	**Inlet**		**Stream**	**Outlet**	
L_5	**$\%X^{mass}$**	**Mass flow**	**R_1**	**$\%X^{mass}$**	**Mass flow**
		(g)			(g)
C_2H_5OH	29.71	4899			
H_20	70.23	11583	H_2	6.67	1100
			H_2O	42.58	7022
			CO	4.49	740
			CO_2	42.84	7065
			CH_4	3.43	565
Total	100	16492		100	16492

Tab. 3.1 Stream compositions and mass flows

Furthermore, I calculate the percent yield which is ratio of actual yield to theoretical yield. Actual yield was basically the amount of product actually produced whereas the theoretical yield is the calculated or expected amount of product. Since, CO Yield = 1, so the Actual CO moles according to yield are calculated by multiplying yield with theoretical Moles of CO which are 34 mols. As per the balanced chemical equation**;** Number of moles of CH_4 was the number of moles of CO produced following ratio of 1:1 and can be calculated by using the following expression:

Moles of CO in product = inlet moles + actual moles = 60mols

I also completed the material balance on all major components of the process which included water gas shift reactor ($wgsr_1$), water gas shift reactor ($wgsr_2$), water separator and fuel cell. As for the overall process material balance the input mass flow must be equal to output mass flow. I converted all the calculated data in the form of a table in order to provide better presentation in the project report which also helps in easy understanding of the entire material balance process and is shown below and it expressed that the overall accumulation during the process is nil:

Input Streams	Mass Flows (gm/hr)	Output Streams	Mass Flows (gm/hr)
Feed	16492	Separator	5345.95
Air to combustor	9886.4	Combustor	10990.4
Air to fuel cell	48864.62	Fuel cell outlet	60010.67
Ethanol to combustor	1104		
Sum	76347.02	Sum	76347.02

Tab. 3.2. Streams mass flow table

CE 3.3.5

Similarly, I carried out the detailed process of energy balance as well. I calculated the energy balance at the pump by using the following formula:

$W_{pump}= V\Delta P$

At Heat Exchanger 1, the energy balance was calculated by me using the following formula:

$Q = mc_p dT$

For the Heat Exchanger 2, the energy balance was computed by me by using the following equation

$Q_c = Hvap + mc_{pdT}$

Since I observed a phase change in this exchanger so heat of vaporization was introduced and the energy balance at heat exchanger 3, 4, 5 and 6 was also computed by me.

For the purpose of computing energy balance at the Molten Salt Reactor (MSR), I made the following calculations and the main reaction is also mentioned as:

$CH_4 + H_2O \rightarrow CO + 3H_2O$

Heat of Reaction = +206 kJ/mole

Operating Temperature = 800 ◦C

$Q= m_{in}c_{pin}\ (25-800) +\Delta H_{rxn} +m_o c_{po}\ (800-25)$

Q= 7843 kJ/hr

I repeated the same steps with relevant formulas and equations to compute energy balance at $WGSR_1$, WGSR2, cooler and fuel cell.

CE 3.3.6

In the next vital stage of the project, the process of detailed equipment design was completed by me in which I initially designed the main component of the project, the reformer. I designed this instrument in such a way in which reforming of the reactants was to be carried out. Steam Ethanol reforming was an endothermic process with heat of reaction as 106 kJ/mol. I observed that the reaction requires a high amount of energy which I figured out to be provided through fuel burning in the outer shell of the reformer. I suggested to complete this procedure with the presence of Ni acting as a catalyst at 500 °C temperature and 5 bar pressure. I used this procedure for the production of pure hydrogen which was to be further used as fuel cell feed where it would react with oxygen to generate power in order to drive the motor of automobile. The main chemical reaction which was taking place in this process was:

$$C2H5OH + 3H_2O \rightarrow 2CO_2 + 6H_2$$

I used the following formula to find the weight of catalyst required for given conversion:

$$\frac{W}{Fao} = \int_{Xo}^{Xf} \frac{dXa}{-ra}$$

Furthermore, the pressure drop was also calculated by me by the use of the following formula:

$$\frac{\Delta P}{L} = \frac{150 V_o \mu (1-\varepsilon)^2}{\Phi_s^2 D_p^2 \varepsilon^3} + \frac{1.75 \rho V_o^2 (1-\varepsilon)}{\Phi_s D_p \varepsilon^3}$$

As for the mechanical design of the reformer, the tubes that I used for Ethanol reforming were designed to have a wall thickness of 0.43 cm and made of chromium nickel metal alloy. The reason for choosing this material for the design by me was that it can sustain a high temperature of 500°C i.e.; the operating temperature of ethanol reformer.

CE 3.3.7

For the purpose of dealing with environmental regulations against CO emissions which is a greenhouse gas so Water Gas Shift Reactor was suggested to be used by me as it was mainly used where there is production of Caron Monoxide (CO). The reaction is exothermic and 41kJ/mol of energy is liberated. WGS reaction always takes place in two steps; High Temperature Shift (HTS), Low Temperature Shift (LTS). As the reaction is exothermic and more favorable at low temperature, sonearly 70% conversion was achieved in HTS whereas 90% was achieved in LTS. I suggested the use of Cu(55%), ZnO(30%), Al_2O_3(15%) as catalyst in the process of WGS.

CE 3.3.8

Within the next phase of the project, it was required for the designed processes and equipment to be analyzed by the use of software analysis tool so as to understand its operation in a better way and rectify if there were any problems. For this purpose, I simulated each and every aspect of the process using the Aspen HYSYS V10 software. I entered all the specifications and designed details of the reformer in the dialogue box of the software shown below:

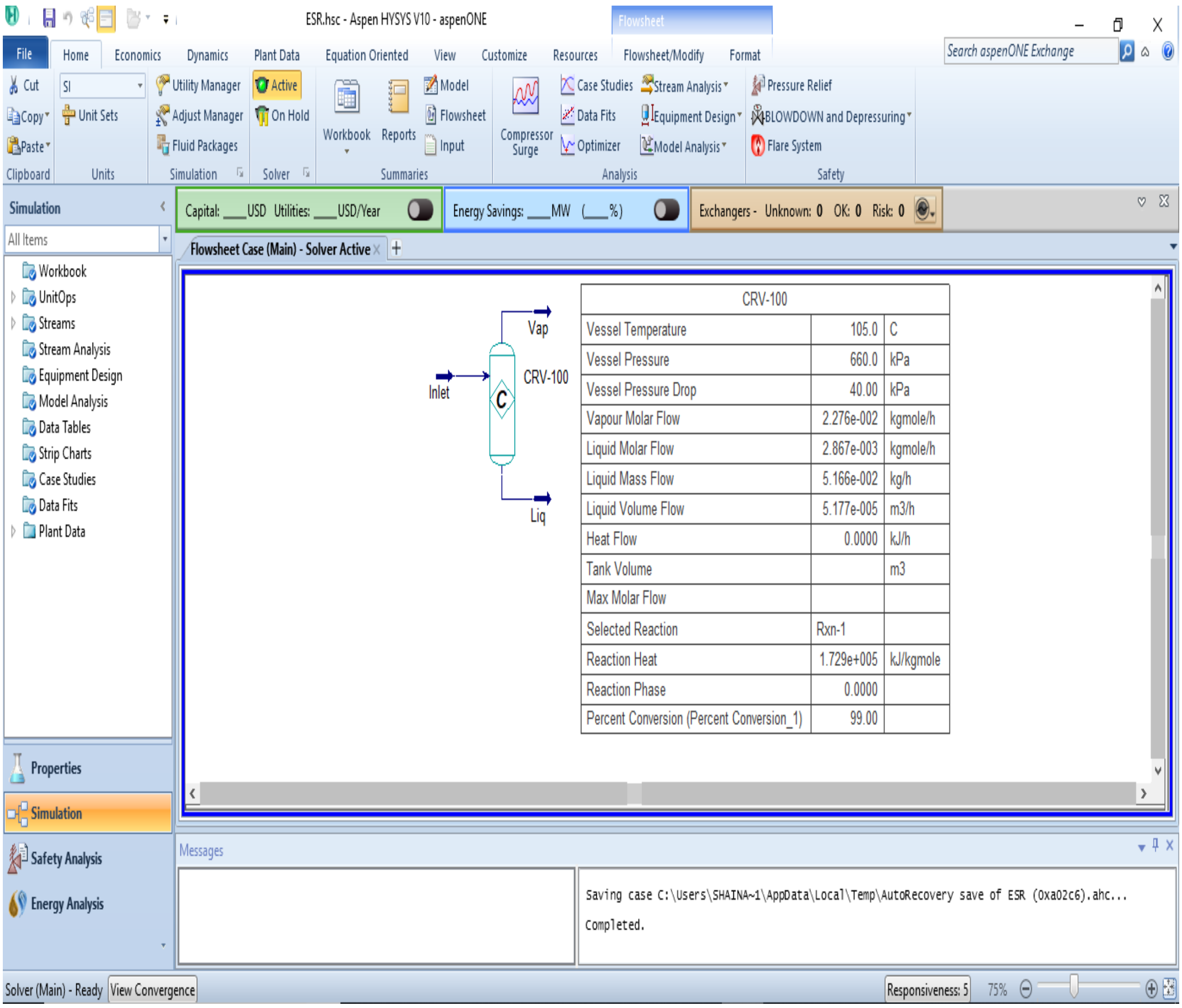

Fig. 3.3. Ethanol Reformer design details in Aspen HYSYS V10

CE 3.4 Summary

The challenges I faced during the course of this project, enabled me to understand the complexities of such process in the chemical engineering field and the factors impacting them. It also provided me with an opportunity to develop my skills so as to solve multifaceted engineering problems and devise practical and effective solutions for them. I also completed my project on time and by carrying out regular progress updates and reports to the project supervisor.