

DYNAMICS SIMULATION OF VINYL CHLORIDE MONOMER (VCM)  
REACTOR USING ASPEN HYSYS

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DYNAMICS SIMULATION OF VINYL CHLORIDE MONOMER (VCM) REACTOR USING  
ASPEN HYSYS

MUHAMMAD NOR ASNIZAN B NAWAWI

Thesis submitted in fulfillment of the requirements  
for the award of the degree of  
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FEBRUARY 2013

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**Dedicated to my family and friends**

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I acknowledge my sincere indebtedness and gratitude to my family for their love, dream and sacrifice throughout my life.

## **ABSTRACT**

The purpose of this research is to observe the dynamics simulation of Vinyl Chloride Monomer (VCM) process particularly in reaction section. The simulation is conducting by Aspen Hysys software by applied some steps. To develop dynamics simulation, the first step is developing steady state mode. Once the steady state simulation have completed, then sizing and installing the controller should be done. The third step is tuning of the controller. The characteristics of the reaction process can be investigated by changing of a raw materials flow rate. The result shows that the transient responses of the VCM reactor are inverse response process. The outcome result of this research is the oxychlorination reactor section of vinyl chloride monomer can be develop by using dynamics simulation as the monitoring process if any disturbances occur after the parameter is changed in process meanwhile the environment and safety of human secured from any pollution and dangerous incident. Apart from that, this study can become guidance to VCM industry to improve process performance. The significant of the study is improving knowledge of the characteristic of VCM process in reactor section by simulating process using dynamics simulation. Another significant is commercialization of dynamics simulation to VCM industries that bring 1001 benefit to industries.

## ABSTRAK

Tujuan kajian ini adalah untuk memerhati process simulasi dinamik vinil kloride monomer terutamanya di dalam seksyen reaksi. Simulasi dijalankan oleh perisian Aspen Hysys dengan menggunakan beberapa langkah. Untuk membangunkan simulasi dinamik, langkah pertama adalah membangunkan mod keadaan stabil. Setelah simulasi keadaan stabil telah selesai, maka saiz dan memasang kontroler perlu dilakukan. Langkah ketiga adalah mengawal kontroler. Ciri-ciri proses tindak balas boleh disiasat oleh perubahan kadar aliran bahan-bahan mentah. Hasilnya menunjukkan bahawa tindak balas sementara reaktor VCM adalah proses tindak balas songsang. Keputusan hasil kajian ini adalah seksyen oxychlorination reaktor vinil klorida monomer boleh dibangunkan dengan menggunakan simulasi dinamik sebagai proses pemantauan jika sebarang gangguan berlaku selepas parameter berubah dalam proses. Sementara itu, alam sekitar dan keselamatan manusia dipelihara daripada sebarang pencemaran dan kejadian berbahaya. Selain daripada itu, kajian ini boleh menjadi panduan kepada industri VCM untuk meningkatkan prestasi proses. Signifikan kajian meningkatkan pengetahuan tentang ciri-ciri proses VCM dalam seksyen reaktor oleh simulasi proses menggunakan simulasi dinamik. Satu lagi kesan yang ketara adalah pengkomersilan simulasi dinamik kepada industri VCM yang membawa 1001 manfaat kepada industri.

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## LIST OF ABBREVIATIONS

PVC	Poly Vinyl Monomer
VCM	Vinly Chloride Monomer
SP	SetPoint
OP	Output Signal
PV	Process Variables
EDC	Ethylene dichloride/ 1,2-Dichloroethane
OSHA	Health and safety regulations
PPM	Part per Million
HCl	Hydrogen Chloride

## **CHAPTER 1**

### **INTRODUCTION**

#### **1.1 BACKGROUND OF RESEARCH**

Vinyl chloride is the organic chloride that most important in industrial chemical used to produce the polymer polyvinyl chloride (PVC). The chemical compound 1,2-dichloroethane or ethylene dichloride (EDC), is a chlorinated hydrocarbon, mainly used to produce vinyl chloride monomer (VCM,) EDC is a colourless liquid with a chloroform-like odour. VCM and EDC are very harmful substances where both this substances is toxic and flammable, then the manufacture of VCM and EDC should concerns regarding to hazard, safety and pollution. The required development the software of chemical process gives significant impact in chemical process simulation. With the small number of VCM industry that using the simulation on their process, this research will bring the opportunity to industry where dynamic simulation can be one tool to reduce plant design time by allows

designer to quickly test various plant configurations without effect the society and environment. A process simulation also displays significant features and characteristics of the system which one wishes to study, predict, modify or control. It also represents some dynamic system be use to gain important information when the costs, risks or logistics of manipulating the real system in plant are prohibited. Therefore this research is important to industry prove to society that the modern VCM industry is more safety and cleanest.

## **1.2 PROBLEM STATEMENT**

The increasing of polyvinyl chloride (PVC) gives impact to increase of production of vinyl chloride monomer (VCM). VCM is produced from the exothermic reaction. The raw materials of production VCM is ethylene, chlorine and oxygen where all the material is 100% pure. As an exothermic reaction, it will give the biggest problem that is runaway reaction in process. Besides that two from raw material which ethylene and oxygen are flammable and toxicity substance. Thus, a dynamics simulation representation consistent with the actual plant needs to be developed as a benchmark for chemical process engineers to improve the performance of the process. Then the hazard effect to people, environment and properties can be avoided.

### **1.3 RESEARCH OBJECTIVE**

The objective of this research is;

1. To develop dynamics simulation of VCM process (reaction section) using Aspen Hysys software.
2. To provide troubleshooting guideline before applied into actual plant.

### **1.4 RESEARCH QUESTION**

The research question that will obtain from this research is:

1. How to develop dynamics simulation of VCM process (reaction section).
2. Can dynamic simulation of VCM process provide a benchmark to chemical engineer to improve the performance of the process?
3. Can dynamics simulation provided the troubleshooting occur in VCM process?

## **1.5 SCOPE OF STUDY**

The scope of the researches is the dynamics behavior on VCM in reactor section that require specific operating procedure to ensure the reaction process is stable. In addition for scope of software for dynamic simulation is ASPEN HYSYS.

## **1.6 EXPECTED OUTCOME**

From the study, the vinyl chloride monomer (VCM) can be demonstrated using dynamics simulation. The result of this study can become guidance to VCM industry to improve process performance and safety.

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## **1.7 SIGNIFICANCE OF STUDY**

The significant of the study is improving knowledge of the characteristic of VCM process by using dynamics simulation. Another significant is commercialization of dynamics simulation to VCM industries.

## **1.8 CONCLUSION**

This study is highly beneficial and most helpful research for industries to analysis any question or problems that related to abnormal of process production VCM in reactor section using dynamics simulation to obtain quality and quantities product without effect on environment, property, human safety and organization cost. Investigate ways to support the integration of representation, guidance, simulation and execution capabilities for models of software processes.

## **CHAPTER 2**

### **LITERATURE REVIEW**

#### **2.1 INTRODUCTION**

The purpose of this chapter is to provide a literature review of past research effort such as journals or articles related to reactor section and dynamics simulation analysis for production of vinyl chloride monomer (VCM). Moreover, review of other relevant research studies are made to provide more information in order to understand more on this research. Health and safety regulations (OSHA) require the monitoring of concentrations of hazard species in all facilities where VCM is produced or used. The time for person can be in environment that exposed to less than 1 ppm is over 8 hours and cant exceeding 15 minute for no more than 5 ppm environment. Exposures to more than 100 ppm can bring to dangerous disease to person. The characteristic of VCM is flammable to heat, flame and oxidizing agent based on fire triangle. The use of stabilizers prevents polymerization during

processing and storage (Alexandre 2008). Dynamics simulation is one tool that plays a significant role in improving product quality, plant efficiency, and safety. The respond that come from the dynamics simulation are useful tool that can be applied to all tasks of process operation to predict the behavior of specific unit or process. Software modularity, user friendly interfaces and computing power has increasingly opened up new opportunities for the application of advanced mathematical models in process operations. In new global competition to produce good quality of VCM, organization need to accelerate process engineering design, reduce capital costs and optimize the various process operations (Kellner et al, 1999).

## 2.2 VINYL CHLORIDE MONOMER (VCM) PROCESS

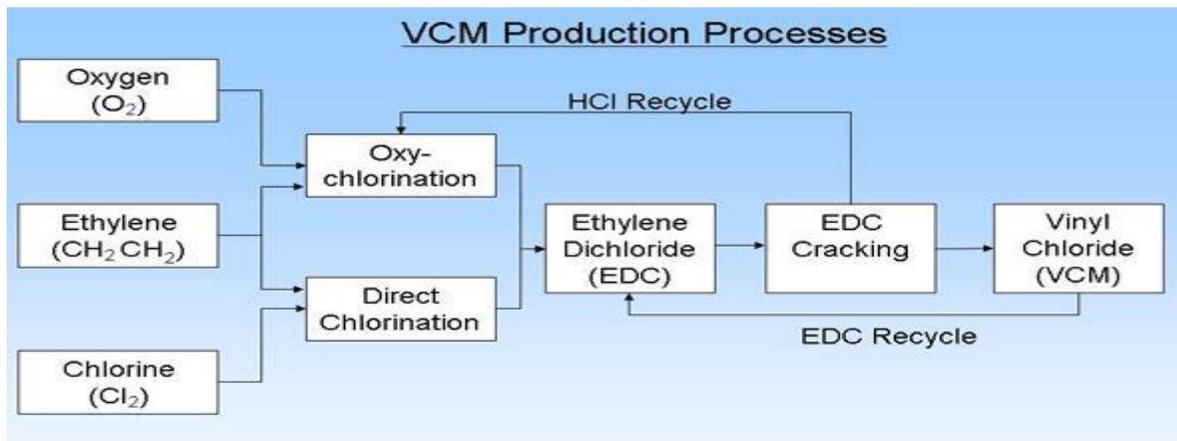


Figure 2.1: Block Diagram of VCM Process

Based on the figure 2.1, Vinyl chloride monomer (VCM) or (CH<sub>2</sub>=CHCL) process is involved 3 sections which reaction section, separation section and purification section. For reaction section, the process that involved is recovery of HCl with oxychlorination process and direct chlorination process. In separation process is thermal cracking (pyrolysis) process and purification section is VCM purification. For this research only oxychlorination process in reaction section been focus where 85% of amount 1,2 – ethylene dichloride (EDC) produce from this process (Alexandre, et,al, 2008). The three main steps process are explained briefly below:

- Direct chlorination of ethylene to 1,2 - ethylenedichloride (EDC):
  - **$C_2H_4 + Cl_2 \rightarrow C_2H_4Cl_2 + 218 \text{ kJ/mol}$**
- Thermal cracking (pyrolysis) of EDC to VCM:
  - **$C_2H_4Cl_2 \rightarrow C_2H_3Cl + HCl - 71 \text{ kJ/mol}$**
- Recovery of HCl and oxychlorination of ethylene to EDC:
  - **$C_2H_4 + 2HCl + 0.5O_2 \rightarrow C_2H_4Cl_2 + H_2O + 238 \text{ kJ/mol}$**

Hence, an ideal balanced process can be described by the overall equation:



### 2.2.1 Oxychlorination process.

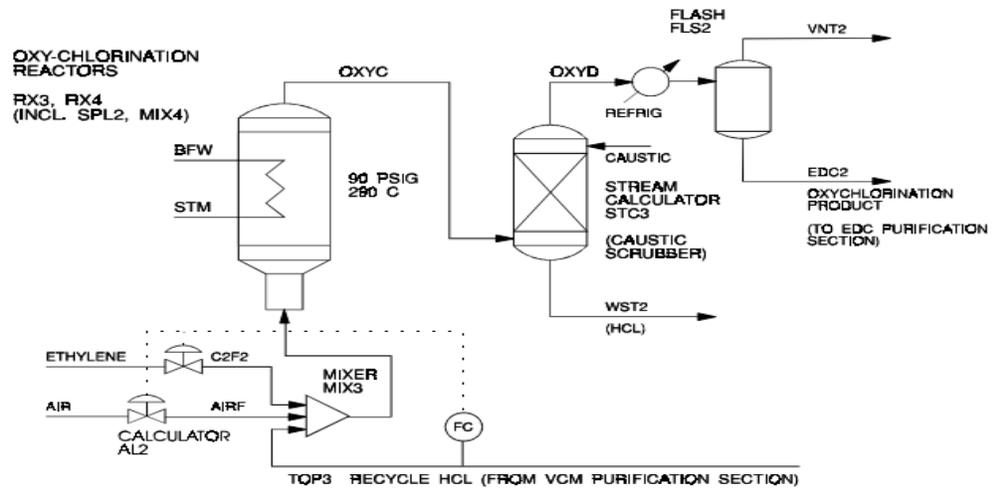


Figure 2.2: Process Flow Diagram For Oxychlorination Process

The term of oxychlorination describes a process whereby chlorination usually of hydrocarbon is achieved with hydrogen chloride and oxygen in the present of catalyst (Magistro et al, 1968). In production Vinyl Chloride Monomer (VCM), oxychlorination is one process in production of where in this process the ethylene, dry HCl and air or pure oxygen is react in a heterogeneous catalytic reaction to form EDC and water. The reaction such as:

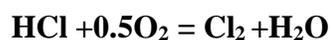
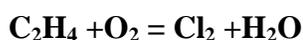


The oxychlorination of ethylene to EDC and water is conducted in the gas phase at specify parameter such temperature in range between 200-300° C and pressure between 2-4 bar in fixed - bed reactors or fluid - bed reactors. The fluid - bed technique offers more

intensive heat transfer, prevents the occurrence of hot spots and allows more efficient catalyst regeneration. Function of fluid bed reactor is by improve contact two phases in a chemical process and is used to store heat in chemical process. The excellent distribution in fixed-bed makes it possible to maintain a constant temperature to ensure low by-product formation and to achieve optimum process control. The reaction gas passes a filter unit in which the catalyst fines are separated from the gas.

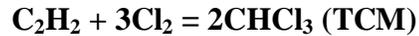
From this reaction the conversion of EDC can achieved with selectivity between 91 – 96% from the ethylene conversion of 93 – 97%. An increase in by-product formation is observed with increasing reactor temperature. The oxychlorination reaction is exothermic reaction where heat capacity is -238 kJ/mol EDC made) and requires heat removal for temperature control, which is essential for efficient production of EDC. Higher reactor temperatures lead to more by-products, mainly through increased ethylene oxidation to carbon oxides and increased EDC cracking yield VCM and cracking steps lead progressively to by-products with higher levels of chlorine substitution. The  $\text{CuCl}_2$  serves as catalyst often contain activators and stabilizers such as chlorides of the rare earths and alkali metals. Under the reaction condition is no free chlorine (Wakiyama, 1971). Catalyst also deactivate if the temperature is high more than  $300^\circ\text{C}$  though the sublimation of  $\text{CuCl}_2$  increased. The process flow diagram is like in figure 2.1. Ethylene, oxygen and recycle HCl will mix first in mixer before entering the reactor section. The product from reactor section will enter caustic scrubbing tower where unreacted HCl is removed. The vapor then passes to a refrigerated condensation system to recover EDC and water. The product steam is cooled and flashed to remove all non condensable mainly nitrogen and unreacted oxygen at top product and EDC at bottom product before the EDC flow to purification section.

Some key impurities are listed below: 1,1,2 - trichloroethane (TCE), chloral (CCl<sub>3</sub> - CHO), trichloroethylene (TRI), 1,1 - and 1,2 - dichloroethylenes, ethyl chloride, chloro - methanes (methyl -chloride, methylen - chloride, chloroform), as well as polychlorinated high – boiling components (Alexandre et al, 2008). In particular, chloral needs to be removed immediately after reaction by washing because of its tendency to polymerization. The formation of TRI is undesired, because its removal by distillation is very difficult. In fact, TRI and EDC form a low - boiling point azeotrope very close to EDC. The formation of TRI in the oxychlorination reactor is due to the acetylene entrained with the HCl byproduct from cracking. Secondary reactions manifest, as explained next. An amount of ethylene is lost by combustion at higher temperature:



Chlorine is involved further in radical reactions producing many chlorinated species. At higher temperature even the C – C bond in chlorinated products can break, forming chloromethanes (Alexandre et al, 2008). All these reactions lead finally to a wide spectrum of impurities. Stoichiometric equations are given below and may be used for material - balance purposes, although the true reaction mechanism is much more complex:





### 2.3 DYNAMIC SIMULATION

In industry of VCM, redesign and optimization of existing process is required to produce the quality product. To overcome the problem, dynamic simulation is needed for all engineers as well as by other operational groups is highly desirable. By applied the dynamics simulation into VCM production, the whole plant can be described into dynamics model for purpose to address a variety of abnormal issues from the process, and to supporting process improvements,

In many cases, simulation is an aid to decision making. It also helps in risk reduction and helps management at the strategic, tactical and operational levels. There has a reason for engineer to use the dynamics simulation into real plant. First purpose is control and operational management. For these advantages simulation can also provide effective support for managerial control and operational management. Simulation can facilitate project tracking and oversight because key project parameters such actual status and

progress on the work product, raw material consumption and etc can be monitored and compared against planned values computed by the simulation. This helps personnel determine when possible corrective action may be needed. The major activity of support operational decisions such coding and integration testing can be commencing by using simulation. Evaluating current project status using timely project data and employ simulation to predict the possible outcome if proposed actions such commence integration testing can be taken or delay can be due by personnel (Kellner et al, 1999). Another purpose is process improvement and technology adoption from organization plant in a variety of ways. In process improvement settings, organizations plants are often faced with many suggested improvements. Advantage of dynamics simulation is simulation can provide specific process improvement decisions such as go/no go on any specific proposal, or prioritization of multiple proposals by forecasting the impact of a potential process change before putting it into actual practice in the organization.

Finally, the advantage by using dynamics simulation in VCM process is training through involved in simulations can help people to accept the uncertainty of their initial prediction about the results of given actions in process. There has two type of person where one has abilities to predict from data and one do not possess good skills or inherent abilities to predict the behavior of systems with complex feedback loops and/or uncertainties as are present in software processes. Overall, active participation in a good mix of simulations can provide learning opportunities to personnel that could compare real world experience that only be gained through years in industry (Kellner et al, 1999). The developed software tools support the application of model-based approaches to the design, operation, optimization, and control of polymerization processes. Ideally, such a model can predict the

steady-state and dynamic behavior of a process over a wide range of operating conditions to an acceptable degree of accuracy (Krallis et al, 2010).

For the reactor in Aspen Hysys, all of the reactor operations share the same basic property view. The primary differences are the functions of the reaction type (conversion, kinetic, equilibrium, and heterogeneous catalytic or simple rate) associated with each reactor. As opposed to a separator or general reactor with an attached reaction set, specific reactor operations may only support one particular reaction type. For instance, a conversion reactor will only function properly with conversion reactions attached. If you try to attach equilibrium or a kinetic reaction to a conversion reactor, an error message will appear. The gibbs reactor is unique in that it can function with or without a reaction set. Conversion reactors can be used to quickly calculate reaction products. The conversion of a specified reactant is described by an equation which can be a function of temperature. A conversion reactor might be used in place of a plug flow reactor with multiple reactions inside a recycle loop in order to save time. The actual plug flow reactor calculations would be done once the recycle is converged and conditions are more finalized. Another situation where conversion reactors are useful is when product yields are known but detailed kinetics may not be available. Many refinery reactors, including hydro treating, alkylation, catalytic cracking, coking, and others can be modeled with conversion reactors. Another reason for the conversion reactor been used in this simulation is because conversion reactor is a basic for the fluid bed reactor.

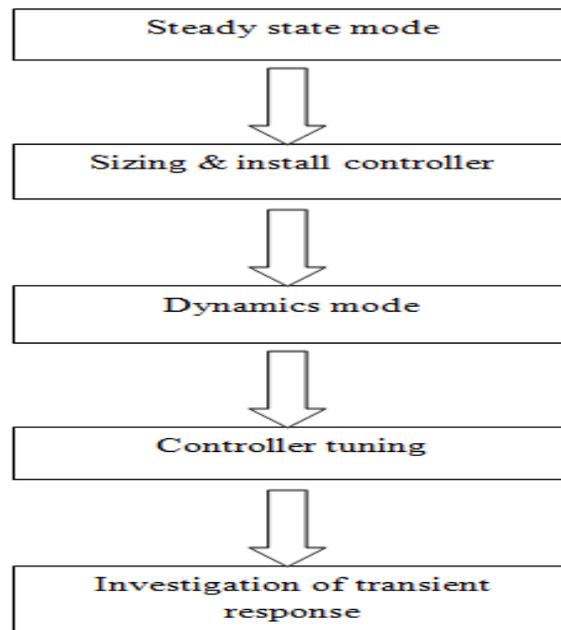
## **CHAPTER 3**

### **METHODOLOGY RESEARCH**

#### **3.1 INTRODUCTION**

In this chapter all step to running the VCM process in dynamics simulation will be describe. First of all the simulator should be easy to use for personnel although the actual modeling task may be carried out by a modeling expert. It is important that the simulation can be run even without a detailed knowledge of the system equations. Furthermore, the implementation of minor changes in the model section such as variations in operating conditions and connectivity between units and the performance of sensitivity studies should always be a relatively simple task. In general, at least as a first attempt the process description by using standard library models rather than setting up an ad hoc model is good practice to adapt (Bezzo et al, 2004). Besides, the training of plant engineers is more effective if approached in terms of unit blocks without moving into the complicated field of

advanced process modeling. Indeed, the modeling activity should not go beyond the connection of different unit operations and the specifications of their operating conditions. From this point of view; the interface should allow a clear representation of unit operations, in terms of model characteristics and input=output declarations. The important issue concerns the dynamic simulation. This should be easy to run and to derive from the steady state model. Ideally, the same tool should be able to perform both the steady-state and the dynamic simulation without changing the simulation environment (Bezzo et al, 2004). Once the modeling specifications have been fulfilled, the simulator should be easily switched from a steady-state to a dynamic representation of the events.



**Figure 3.1: Procedure of dynamic simulation of VCM process (reactor section)**

## 3.2 PROCEDURE

The characteristic of the VCM plant model and the detailed data and specification of the main processes should be collected and obtain from journal and article that related to reactor section of VCM process. The process flow sheets of the simulated VCM plant in HYSYS including the main reactor are shown. The flow sheet process should be described as real as in the real plant (Bezzo et al, 2004). This will greatly facilitate the understanding of the simulation process as well as the critical evaluation of the results deriving from it. The kinetic model that be used in this research is the Peng Robinson property to calculate the physical properties of developed VCM flow sheet a steady state model was built. The Peng Robinson property is selected as it is highly consistent on predicting physical properties of most hydrocarbon based component over a wide range of operating condition. The model may be described in a visual or textual form. Visual models have become the norm for software process simulations because they promote understandability and ease of development. These tools often include an ability to animate the model during simulation to show the flows of objects such as problem reports through the process, the activities currently being performed and so forth. Then the steady state simulation was built. The reactors are modeled as conversion reactor where personnel have change from the actual reactor (fixed bed reactor) because all reactors are functional conversion reactor. Therefore these study will be more interesting while the reactor kinetic are modeled with available standard Arrhenius Kinetic expressions on HYSYS plant with the provided kinetic data. Although the basis for the development of a dynamic model is the steady-state one, a

number of parameters such as temperature, pressure, flow rate, molar flow rate and etc need to be specified in order to run a dynamic simulation. In fact, although available simulators allow including several detailed calculations such pressure losses due to friction, heat exchanger dynamics, pump and valve characteristic equations, etc, too detailed a model may result impractical to run in a reasonable time at the plant level.

In order to conduct dynamic simulation, all equipment must be sized. This sizing does not have to include all the detailed mechanical design. At the conceptual design level, we only need to have approximate estimates of equipment volumes. In the following sections, we discuss the rough-cut sizing of some of the most important unit operations. The sizing calculation gives us a rough idea of the size of the reactor which is accurate enough for dynamic control studies. Pumps, compressors and valves must be positioned and sized to provide the required variations in process flowrates.

Aspen HYSYS is one type of dynamics simulator that's sharing the same physical properties and flowsheet topology as like steady state model. The dynamics simulation uses a different set of conservation equation that account for change occurring over time. Within the dynamics model, an advanced method of calculating the pressure and flow profile of the simulated model is used as the user states the required number of pressure flow specification. The equation is solved simultaneously to find the unknown pressure or flowrates. The developed dynamics simulation of highly integrated plant enables the personnel to understand the interaction within the entire plant and provided great opportunity in testing and studying the developed control strategic and many other operational aspects. Because the scope is the definition of an easy-to-use model that can be used by plant engineers to check the process behaviour and to improve process operation

and control, numerical stability and ease of manipulating the model are requirements as important as the model capability of capturing the fundamental process dynamics. The next step is installing controller in model. The controller such as temperature, pressure, flow rate and another controller may be used to upgrade the process to become more effective and valuable. The connectivity controller to equipment must be arranged perfectly to avoid the uncertainty result. In addition, the tuning of controllers also has to give attention in this research. Because from the tuning the controller, the process will show the personnel either the parameter that personnel set is right or wrong. The result from tuning controller will provide in transient respond type. Lastly the transient respond will be analysis to provide the solution for every problem that occurs in reactor section.

### **3.3 STEADY STATE ENVIRONMENT**

1. Identify the raw material and product for reaction on oxychlorination reactor.  
Raw material: ethylene ( $C_2H_4$ ) oxygen ( $O_2$ ) and Hydrogen Chloride ( $HCl$ )  
Product material: 1-2 Dichloroethane ( $1-2 C_2H_4Cl_2$ ) and water ( $H_2O$ )
2. Start HYSYS
3. Open a new case by clicking on the blank white page OR use the commands File  
New.  
Press Add button.
4. Press the View button to start adding chemical compounds.

5. Install the chemicals for a oxychlorination reactor: Ethylene, hydrogen chlorine (HCl), oxygen, nitrogen, carbon dioxide (CO<sub>2</sub>), 1, 2 Dichloroethane (EDC), and water (H<sub>2</sub>O). If they are not in the order given below then use the Sort List... button feature.
6. Let's look at one of the components
7. Select Ethylene
8. Click on the View Component button
9. Examine the temperature dependent properties given Tdep page.
10. Notice that the ideal gas enthalpy has been correlated using a 5<sup>th</sup> order polynomial.

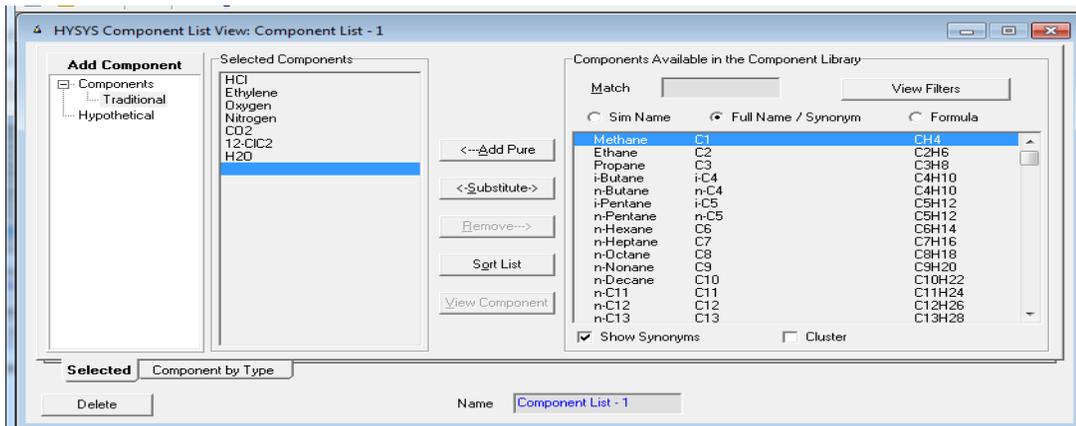


Figure 3.2: Component list

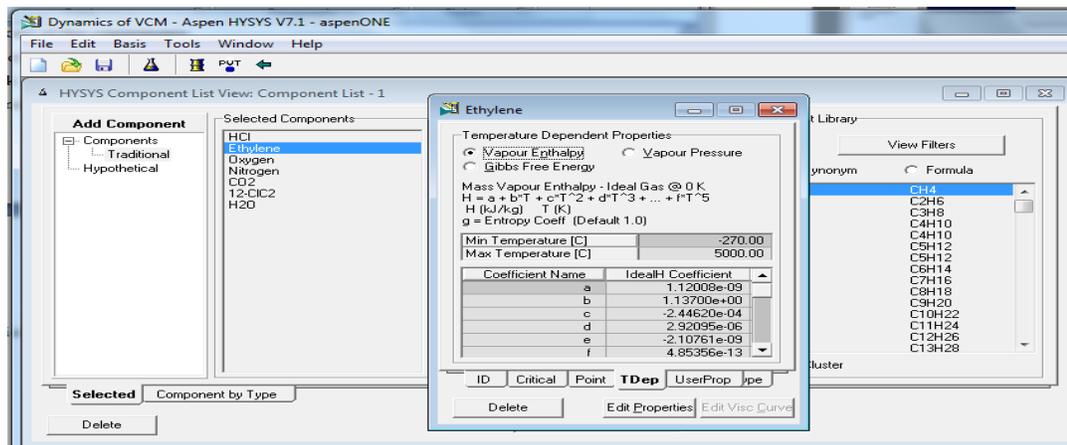


Figure 3.3: Component properties

11. Since these compounds are hydrocarbons, use the Peng-Robinson thermodynamic package.
  - a) Select the Fluid Pkgs menu tab and Press the Add button
  - b) Select the EOS filter radio button to see only Equations of State (EOS)
  - c) Then select the Peng Robinson Equation of State.
  - d) Notice that you have a choice in calculating the enthalpies. You can either use the equation of state – This will be discussed in thermodynamics or you can use a prediction method called the Lee-Kesler Method which is an extension of the Pitzer method. For this tutorial we will use the equation of state method.

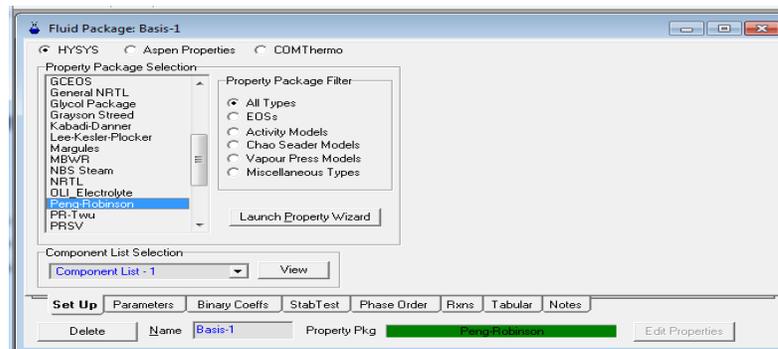


Figure 3.4: Fluid Packages

12. Close the Fluid Package Box and click the button “Enter the Simulation Environment”. After that the PFD box will appear as in figure 3.5

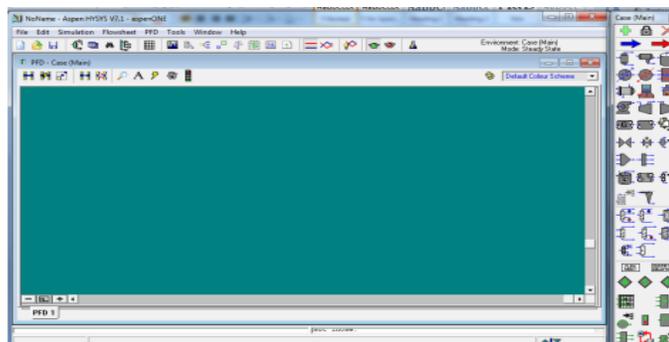


Figure 3.5: Process flow diagram (PFD) box

13. On top bar of PFD box, there has object palette such like picture traffic light. Click it and the case (main) box like right side in like in figure 3.5.

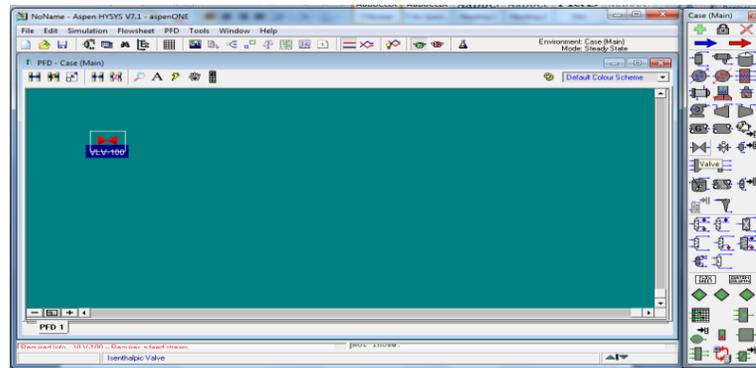


Figure 3.6: Valve flowsheet

14. Click the valve picture and put it into PFD. It will show as in picture above.
15. Click the attach mode in top bar of PFD box. This will help you to attach the stream to the component as in picture below.

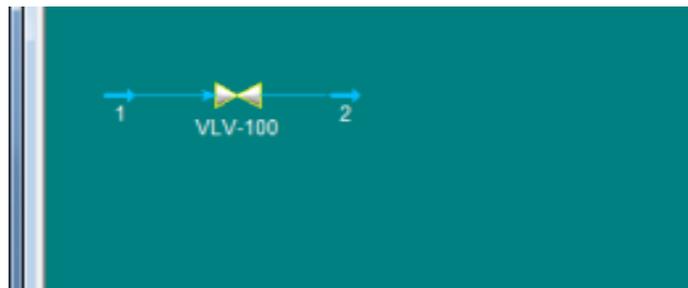


Figure 3.7: Valve & stream flow sheet

16. Then double click on stream no 1. The box properties such as below will pop up and please refer on the box that highlight with yellow colour. This box will help you to fulfill all the condition that the stream need.

17. For the example such figure below. Fill the entire box for the composition table. Click the edit box then another box will appear. You can adjust the composition basic to mole fraction, mass fractions, liquid volume fraction, mole flows, mass flows, and liquid volume flows on the right side. After finish, click ok.

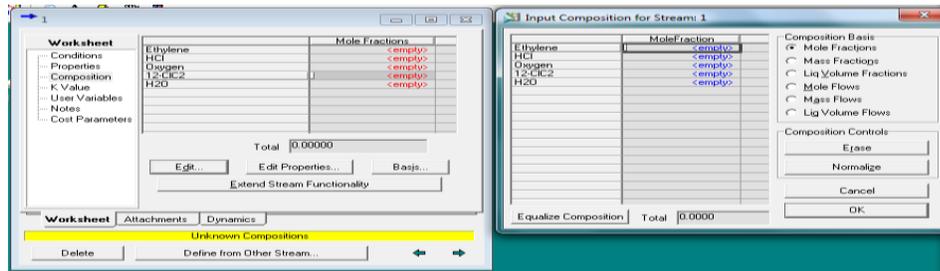


Figure 3.8: Input composition

18. After you have filled the composition, the yellow colour box will suggest you to fill the value for temperature and pressure.
19. Please set temperature and pressure condition until the box below change from yellow to green. That means ok for this stream.

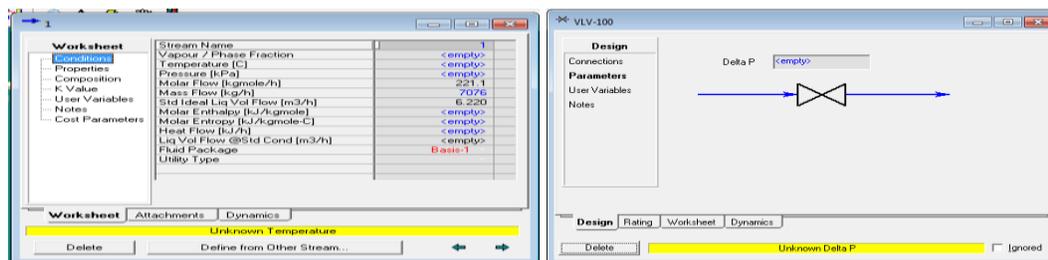


Figure 3.9: Condition & parameter box

20. For the valve, on parameter, personnel need to fill the delta P. This will help the HYSYS to solve all problems to ensure the data of stream 2 is obtained as below. The green colour is stated ok and that means the steady state of HYSYS is success.

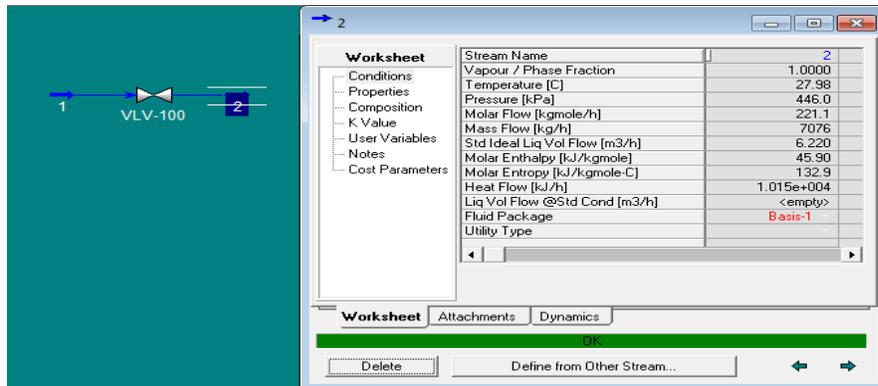


Figure 3.10: Output stream properties

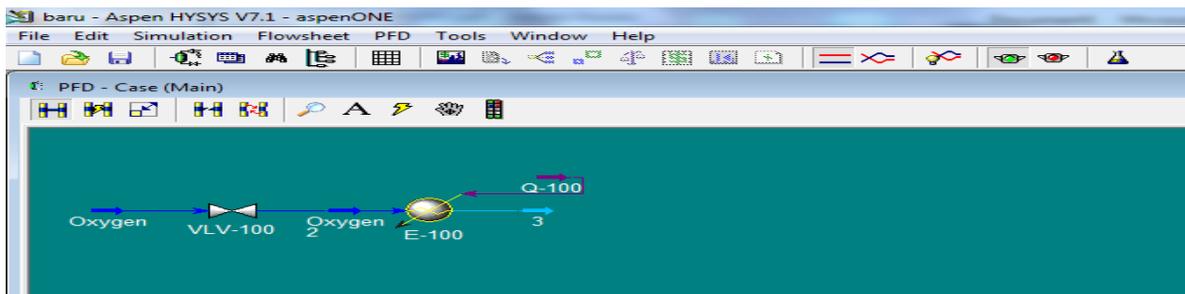


Figure 3.11: Heat exchanger flow sheet

21. The heater item is click from object palette and drag into the PFD box. It will show as in above box. By applied the energy stream on the heater, personnel need fill some item to ensure the stream is in right condition. On parameter item, please fill

up the delta pressure and duty. Then the yellow highlight will change to green. This means the stream can flow.

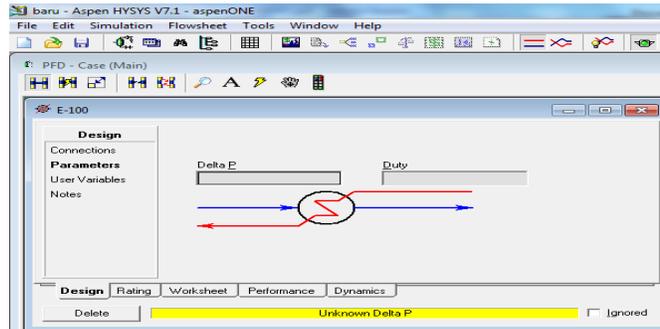


Figure 3.12: Heater properties

22. Continue the stream for ethylene, recycle, and hydrogen chloride same as stream oxygen from starting stream until the stream after heater as figure 3.13. The value for each valve and heater can be obtained in table 3.1.

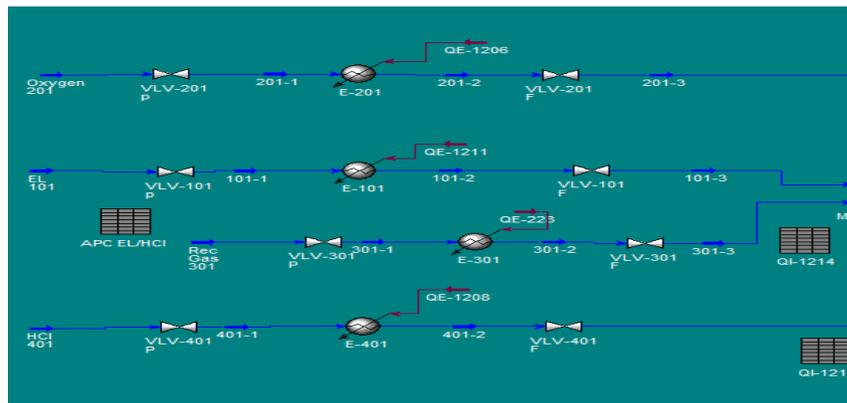


Figure 3.13: Steady state flow sheet

<b>Ethylene stream</b>			
	VLV-101 P (KPa)	E-101 (KJ/h)	VLV-101 P (KPa)
<b>Delta P</b>	648.321	9.601	41.8308
<b>Duty</b>	-	472622	-
<b>Oxygen stream</b>			
	VLV-201 P (KPa)	E-201 (KJ/h)	VLV-201 P (KPa)
<b>Delta P</b>	2821.51	12.89	3.1576
<b>Duty</b>	-	1005000	-
<b>Recycle stream</b>			
	VLV-301 P (KPa)	E-301 (KJ/h)	VLV-301 P (KPa)
<b>Delta P</b>	59.6691	12.20	15.6803
<b>Duty</b>	-	1211810	-
<b>HCl stream</b>			
	VLV-401 P (KPa)	E-401 (KJ/h)	VLV-401 P (KPa)
<b>Delta P</b>	121.749	12.45	15.5522
<b>Duty</b>	-	1829810	-
	VLV-601 P (KPa)	E-501 (KJ/h)	
<b>Delta P</b>	295.233	12.00	
<b>Duty</b>	-	12.45	-

Table 3.1: Properties for valve & heater for each stream

Property	301-1	301-2	301-3	HCl 401	401-1	401-2	401-3
Temperature [C]	30.00	27.99	100.1	100.0	23.00	-13.80	38.17
Pressure [kPa]	1101	445.7	435.7	401.8	3251	430.0	417.1
Molar Flow [kgmole/h]	222.1	222.1	222.1	222.1	437.1	437.1	437.1
Mass Flow [kg/h]	7104	7104	7104	7104	1.227e+004	1.227e+004	1.227e+004
Liquid Volume Flow [m3/h]	6.256	6.256	6.256	6.256	31.99	31.99	31.99
Heat Flow [kJ/h]	1.034e+004	1.034e+004	4.872e+005	4.872e+005	2.191e+007	2.191e+007	2.291e+007
Name	Rec Gas 301	301-1	301-2	301-3	HCl 401	401-1	401-2
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature [C]	50.00	49.78	72.65	72.60	30.00	28.35	96.48
Pressure [kPa]	501.3	441.7	429.6	413.9	551.3	429.7	417.3
Molar Flow [kgmole/h]	1569	1569	1569	1569	885.4	885.4	885.4
Mass Flow [kg/h]	4.630e+004	4.630e+004	4.630e+004	4.630e+004	3.226e+004	3.226e+004	3.226e+004
Liquid Volume Flow [m3/h]	66.03	66.03	66.03	66.03	37.17	37.17	37.17
Heat Flow [kJ/h]	3.851e+006	3.851e+006	5.062e+006	5.062e+006	-8.149e+007	-8.149e+007	-7.966e+007
Name	** New **						
Vapour Fraction							
Temperature [C]							
Pressure [kPa]							
Molar Flow [kgmole/h]							
Mass Flow [kg/h]							
Liquid Volume Flow [m3/h]							
Heat Flow [kJ/h]							

Figure 3.14: Workbook window

23. For enter the input of the stream, personnel can do by click the tool button on top bar and choose workbook. The blue colour is input that personnel can change.
24. For next step is by applied the mixer to combine all of 4 stream to become 1 stream that feed into reactor.
25. For the mixer, click the mixer figure from object palette in PFD window. Double click on the mixer to enter the value for make the mixer be operate.
26. For stream ethylene and recycle, the both of stream is feed into one mixer (mixer 1), then the stream out of mixer 1 will feed the second mixer together with the hydrogen chloride stream. The stream out of mixer 2 will feed together along the stream oxygen into mixer 3. Therefore in this simulation, there have 3 mixers for combine 4 streams before feeding into the reactor.

27. For mixer, personnel are fill the inlets stream box and outlet stream. Then click parameter to change into equalize all.
28. For the stream out of mixer 1, the heater is applied to increase the temperature before the stream entering the second mixer.

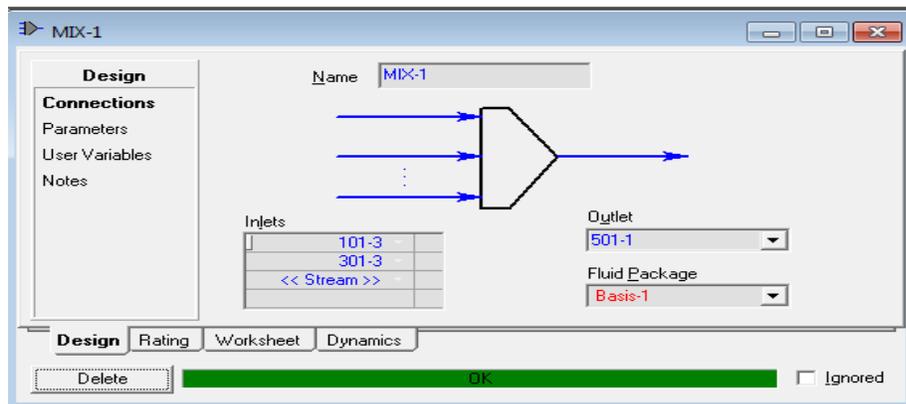


Figure 3.15: Mixer properties

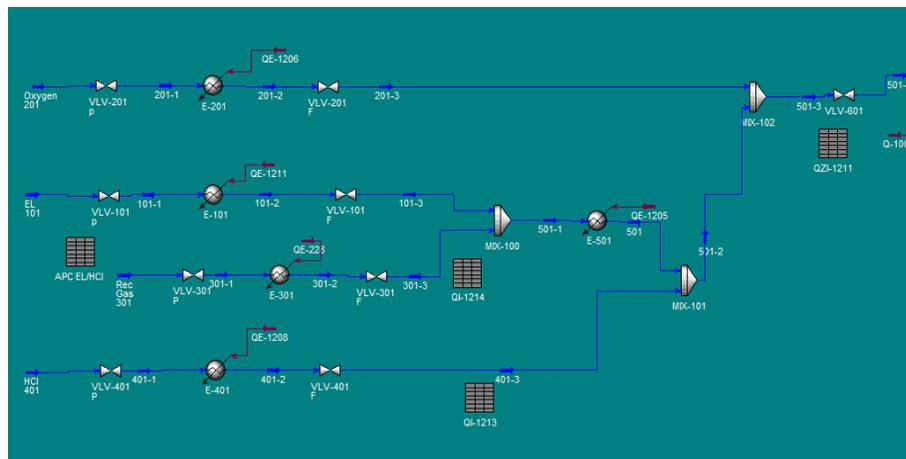


Figure 3.16: Steady state flow sheet

29. On the top Toolbar select the flowsheet then click on reaction package or another step is by return to the Simulation Basis Manager by click on top toolbar the simulation and choose Enter Basic Simulation or click button on keyboard Ctrl + B.
30. The Reaction Component Selection view will appear.

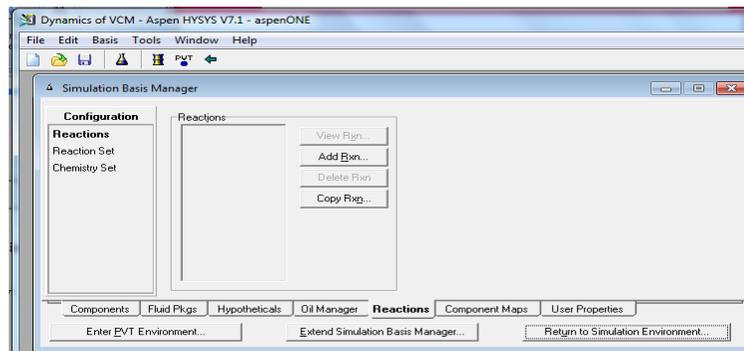


Figure 3.17: Simulation basic manager

31. Press the Add Rxn button in figure 3.18.
32. Reaction window will pop up. Then select the Conversion Reaction. Press Add Reaction.
33. On the Stoichiometry tab add all of the components to the component list by using the drop down list.
34. Select ethylene from the drop down list in the Edit Bar. The Mole Weight column should automatically provide the molar weight of ethylene. In the Stoich Coeff field enter a stoichiometric coefficient based on the reaction. Notice that the coefficient will be negative for reactants and positive for products.

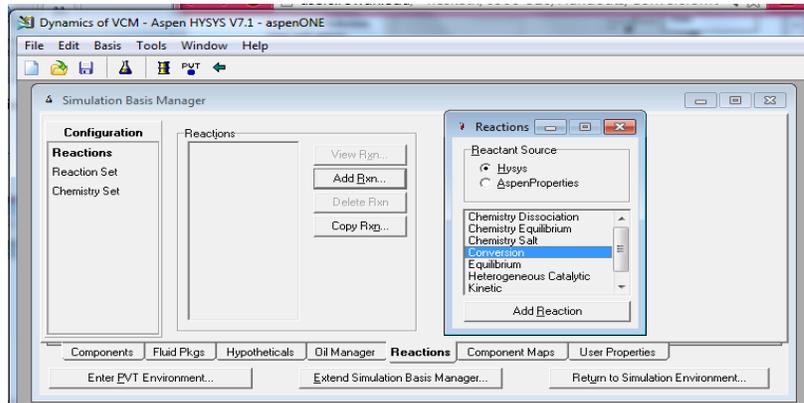


Figure 3.18: Reaction configuration box

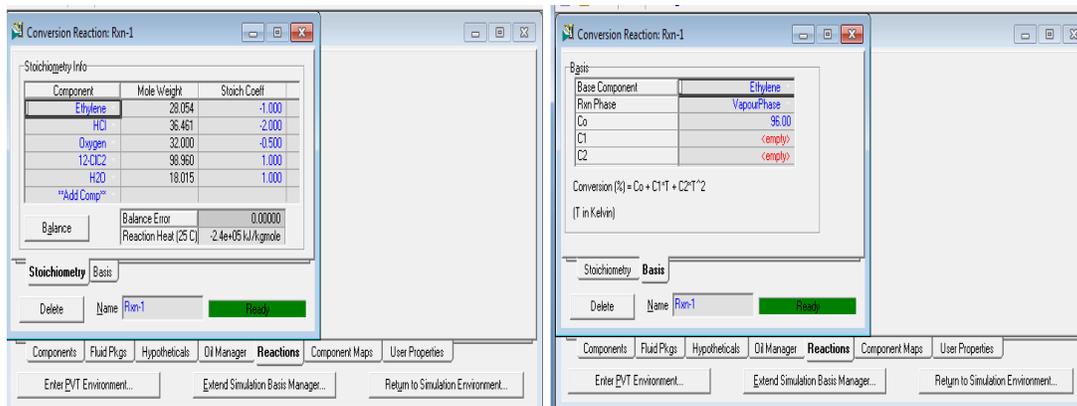


Figure 3.19: Conversion reaction

35. Now define the rest of the Stoichiometry tab as shown in the adjacent figure. Go to Basis tab and set ethylene as the Base Component and Conversion to 96%. The status bar at the bottom of the property view should now show the Ready message. Note that the conversion reaction can be a function of temperature. This is a simple polynomial fit to conversion as a function of temperature data. Using this type of

reaction set we will be able to examine mole and energy balances without knowing the chemical kinetics.

36. Close the property view.

37. By default, the Global Rxn Set is present within the Reaction Sets group when you first display the Reaction Manager. However, for this procedure, a new Reaction Set will be created. Press the Add Set button. HYSYS provides the name Set-1 and opens the Reaction Set property view.

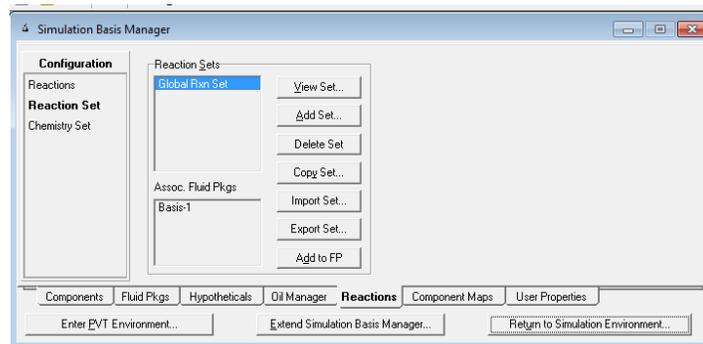


Figure 3.20: Simulation basic manager

38. To attach the newly created Reaction to the Reaction Set, place the cursor in the <empty> cell under Active List.

39. Open the drop down list in the Edit Bar and select the name of the Reaction. The Set Type will correspond to the type of Reaction which you have added to the Reaction Set. The status message will now display Ready.

40. Press the Close button to return to the Reaction Manager.

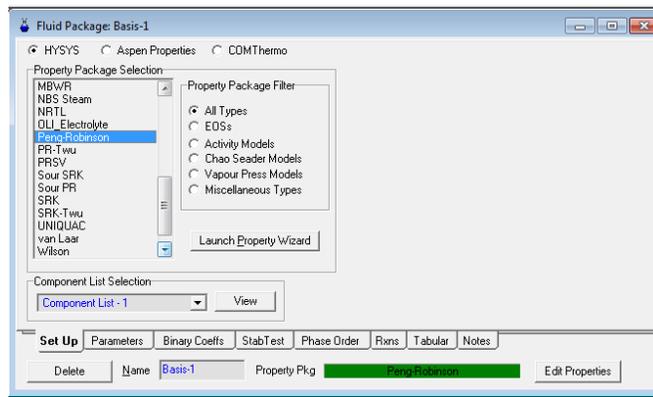


Figure 3.21: Properties package selection

41. To attach the reaction set to the Fluid Package (your peng robinson thermodynamics), highlight Set-1 in the Reaction Sets group and press the Add to FP button. When a Reaction Set is attached to a Fluid Package, it becomes available to unit operations within the Flowsheet using that particular Fluid Package.
42. The Add 'Set-1' view appears, from which you highlight a Fluid Package and press the Add Set to Fluid Package button.
43. Press the Close button. Notice that the name of the Fluid Package (Basis-1) appears in the Assoc. Fluid Pkgs group. The Reaction Set is highlighted in the Reaction Sets group.
44. Now Enter the Simulation Environment by pressing the button in the lower right hand portion.
45. Install a conversion reactor. Either through the
  - a. Flow sheet, Add operation or icon pad.

- b. Click on General Reactors and then a small pad pops up with a choice of 3 reactors. Choose the conversion reactor. Click on the Conversion Reactor icon, then release left mouse button. Move cursor to pfd screen and press left mouse button. Double click on the reactor to open.

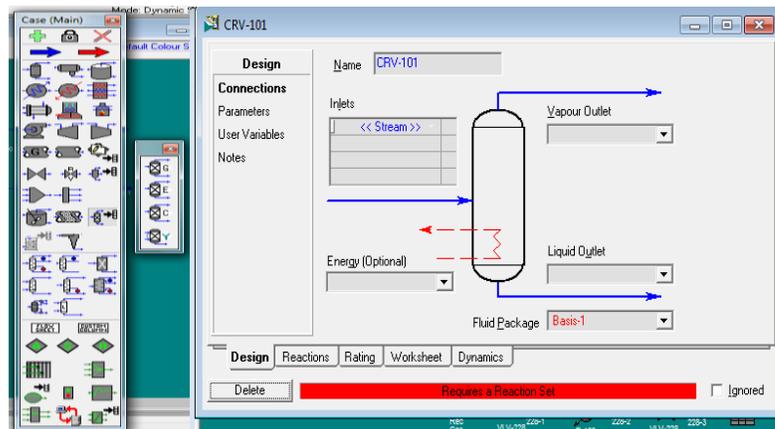


Figure 3.22: Reactor properties box

46. Add stream names and a new reactor name as shown. After naming these streams the following errors appear: Requires a Reaction Set and Unknown Duty.
47. Click on connection at design box on left box. Specify the inject stream, vapour outlet and liquid outlet.
48. For energy, please specify the energy stream that connected to reactor.

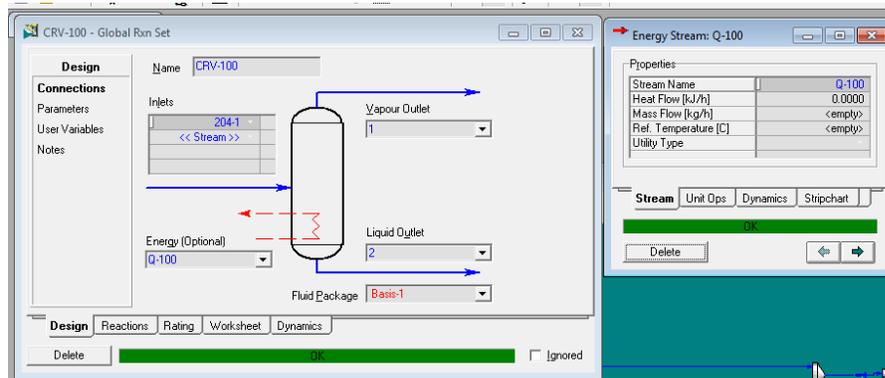


Figure 3.23: Reactor design box

49. Click on reaction and detail to specify reaction set and reaction. Choose the reaction that personnel create on reaction box before.

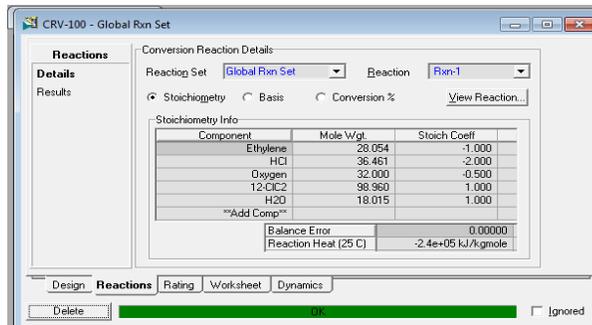


Figure 3.24: Detail reaction box

50. Now run the simulation. For an isothermal reactor specify the outlet temperature.
51. For the adiabatic reactor, delete the temperature specification and specify the heat duty as 0.

52. If you want to check the detail of stream, personnel can click on worksheet at box after you double click on reactor.

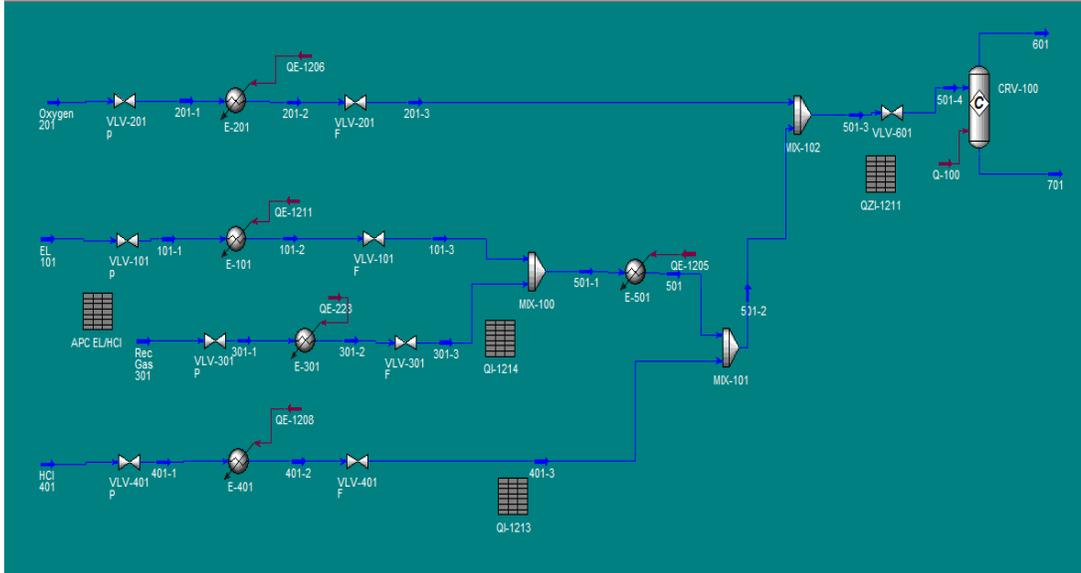


Figure 3.25: Full steady state flow sheet

CRV-100 - Global Rxn Set

Worksheet	Name	501-4	701	601
Conditions	Vapour	1.0000	1.0000	1.0000
Properties	Temperature [C]	118.7	878.6	878.6
Composition	Pressure [kPa]	101.3	101.3	101.3
PF Specs	Molar Flow [kgmole/h]	3073	0.0000	2421
	Mass Flow [kg/h]	9.665e+004	0.0000	9.665e+004
	Std Ideal Liq Vol Flow [m3/h]	139.9	0.0000	107.7
	Molar Enthalpy [kJ/kgmole]	-1.461e+004	-1.855e+004	-1.855e+004
	Molar Entropy [kJ/kgmole-C]	184.1	255.7	255.7
	Heat Flow [kJ/h]	-4.491e+007	0.0000	-4.491e+007
				255.7
				61.06

Design Reactions Rating **Worksheet** Dynamics

Delete OK Ignored

Figure 3.26: Worksheet reactor box

### 3.4 DYNAMICS SIMULATION ENVIRONMENT

1. When the steady state is converged and specified, click the Dynamics Mode on the top tool bar. The dynamics assistant will suggest that some changes be made in some specification so that the flow driven simulation is correctly set up as figure below

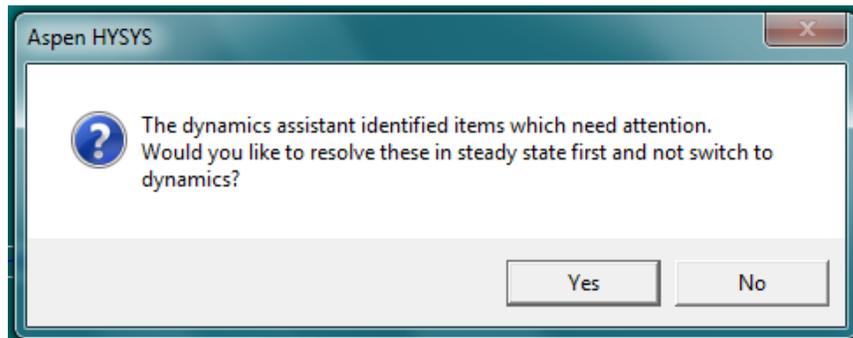


Figure 3.27: Aspen Hysys Assistent

2. This box will appear by click the button stop (arrow 1) as in figure below. Then change the steady state mode to dynamics mode (arrow 2) to adjust the stream follows the dynamics properties. Last is by click back the button start (arrow 3) to start the dynamics mode.

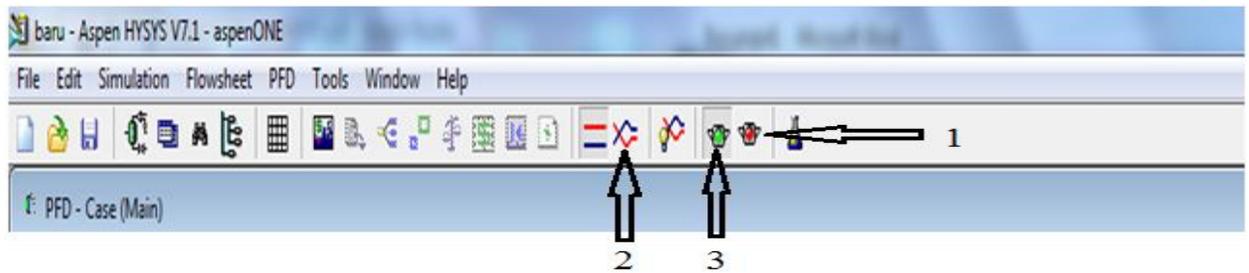


Figure 3.28: Step for dynamics simulation

3. By click the button Yes, another box will appear as Dynamic Assistant Box. Function of Dynamics Assistant is to ensure that a sensible set of pressure flow specification is selected. Hysys will analyzing the case and will recommend a list of changes along with a brief explanation of each group by click at item by display in the list. For serious dynamics work, you will need to make additional changes such as property configuring control system and adding extra equipment and so on.
4. This might be a good place to mention the procedure for switching back to the steady state mode from the dynamics mode. The personnel may want to do this if personnel want to change the structure of the flowsheet or use different equipment sizes or condition.
5. In HYSYS, when the mode is switching from dynamics to steady, it does not return you to the initial steady state condition that personnel had when you originally moved from steady state to dynamics. It recommended personnel to save the steady state condition first before change to dynamics in other file.

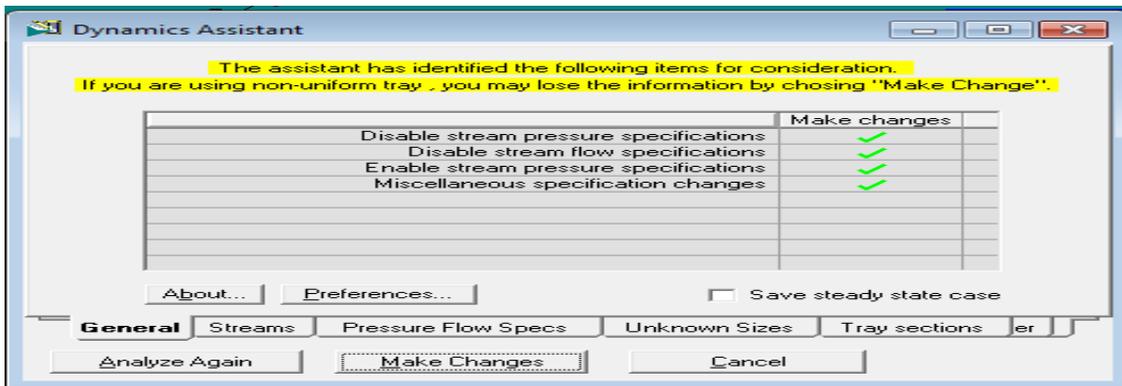


Figure 3.29: List of item in dynamics assistant

6. When personnel has finish read the item in list, personnel need click the button make change to synchronizing the flow with dynamics mode and if the change success the green highlight will appear on top of box. That means personnel steady state mode is work with dynamics mode.

### 3.5 CONTROLLER INSTALLATION & TUNING

1. Click the controller icon on the object pallet and with the right mouse button held down; drag it on the PFD.
2. Double clicking on the controller icon brings up the controller window. The first page tab is connection shown in figure 3.30

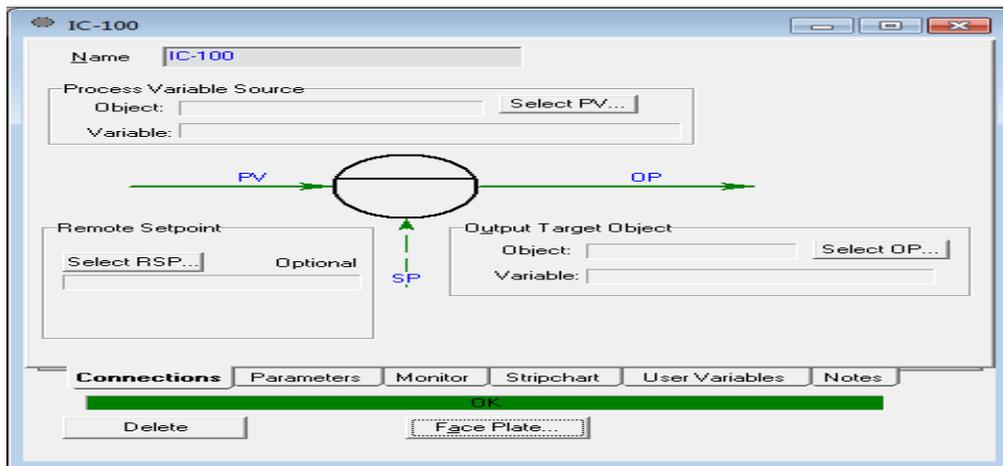


Figure 3.30: Controller properties

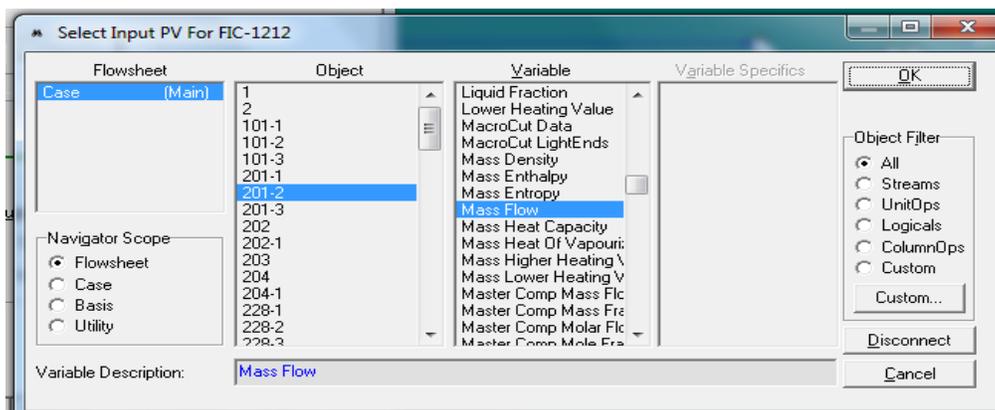


Figure 3.31: PV selection box

- Click the Select PV button to specify the unit or stream and the variables to be controlled. For example to select the PV for the flow controller for the oxygen, we select the stream 201-2 and the variable mass flow as shown in figure 3.31. If a controller is to get an external set point signal, there is a box (Remote Setpoint

Source) in which the source of this signal is specified in cascade arrangement. See figure 3.30

4. Select the target of the OP signal (the place where the controller output signal is sent). Figure 3.32 show the OP signal goes to VLV 201-F with the variable Actuator Desired Position

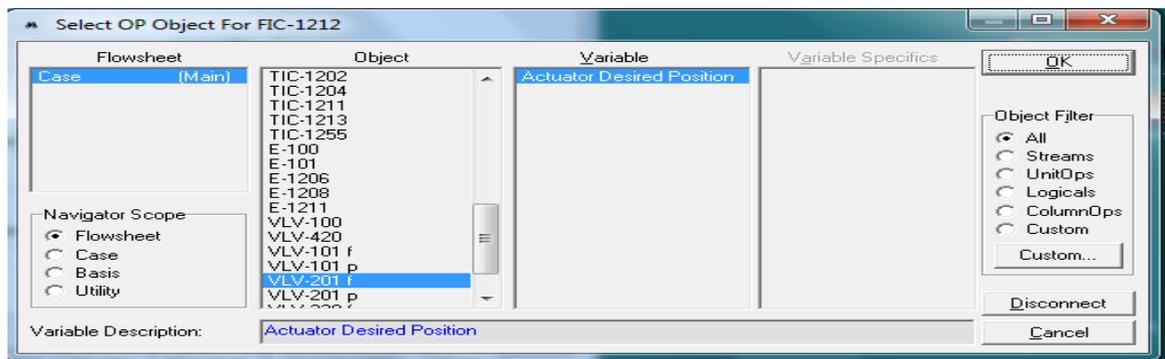


Figure 3.32: OP selection box

5. The second page tab is parameter and is shown in figure above. This is the most important part of the controller specification. In this view you define many of the controller parameter.
  - a) Select the action of the controller (reverse or direct). The flow controller would be reverse acting since an increasing in flow should result in moving the valve 201-F toward the closed position.
  - b) Specify the range of the sensor/transmitter. For the flow controller, personnel should choose a range 0 for minimum PV until twice of mass flow of the stream at steady state for maximum PV. For the pressure controller,

personnel select range from 1 bar until 11 bar because the operating pressure for all stream is around 1-11 bar. For the temperature controller, the range is around -50% and +50% of the steady state condition for each stream.

6. Check the values of the process variables, the setpoint and the percent valve opening. Sometimes the PV signal is not initialized properly until the integrator is started. This occurs in some level loops. When this situation arises, keep the controller on manual until the integrator has been started. Then personnel can change controller to auto.
7. Specify the controller tuning constants: gain  $K_c$ , integral time  $t_I$  and derivative time  $t_D$ . To achieve a proportional only controller, delete whatever number is in the integral box (“empty” should appear).
8. Put the controller into manual or automatic. If the controller receives its set point from another controller, click the “remote” SP Mode button on the connection page tab.
9. The final step is to click the Faceplate button at the bottom of the window. This places a faceplate on the workspace as shown in figure 3.33.

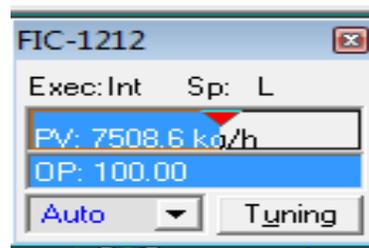


Figure 3.33: Faceplate box

10. The values of the process variables PV and the controller output OP are displayed as horizontal bar chart. To change the set point, when the controller is on automatic, double clicking on the PV display opens a window where you can enter the desired value. When the controller is on manual, double clicking the OP display opens a window where you can enter the desired value of the signal to the valve.
11. The faceplate indicator if the controller is on manual or automatic and the controller can be switched from one to other by using the dropdown arrow, as illustrated in figure, clicking the tuning button on faceplate opens up a window showing the parameters page tab. From this view the tuning constants can be changed.



Figure 3.34: Controller faceplate

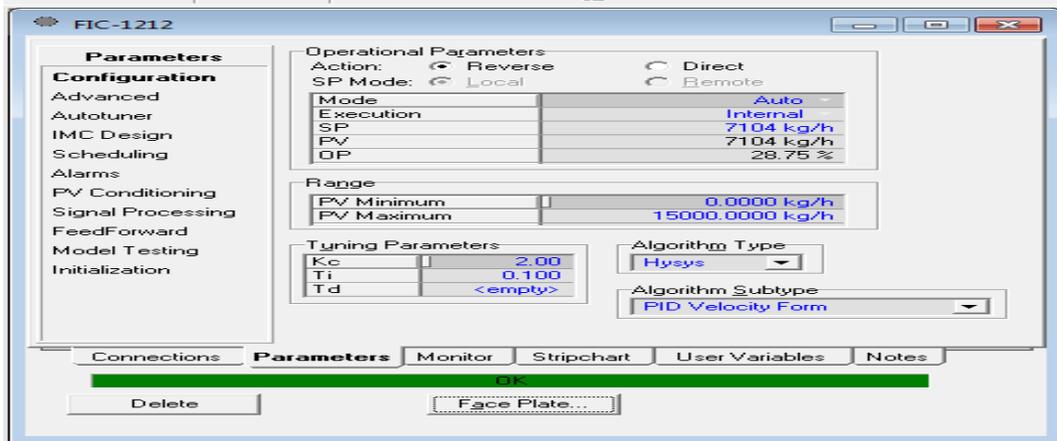


Figure 3.35: Controller parameter

12. In figure 3.35 is the box where personnel adjust the input of the set point (SP) for increasing or decreasing 20% from the stable condition.
13. For the pressure, temperature and flow controller, the step is such above. Only OP and PV that need be entering the stream for each controller.

### 3.6 INVESTIGATION OF TRANSIENT RESPONSE

#### 3.6.1 Installing recorder/ strip chart

1. Personnel need to be able see how variables are changing with time. Strip chart recorder/ data loggers are useful for this purpose.

2. The steps for installing and defining the properties of recorder are by first click Tools on the top menu bar and choose DataBook just like in figure 3.36.
3. On the variables page tab, click Insert. Select the variables to be recorded. For example to record the mass flow of product from the reactor, personnel select under object the “601” stream as shown in figure 3.37
4. Under the variable, personnel choose Master Comp Mass Flow. Then click 1,2 CIC2 in variable specific box. Then click OK button. To add the mass flow for stream 201-3, personnel click Insert again and select the under object stream 201-3. After that under variable click Mass Flow then click OK.
5. Personnel can insert all the variables you want to record.

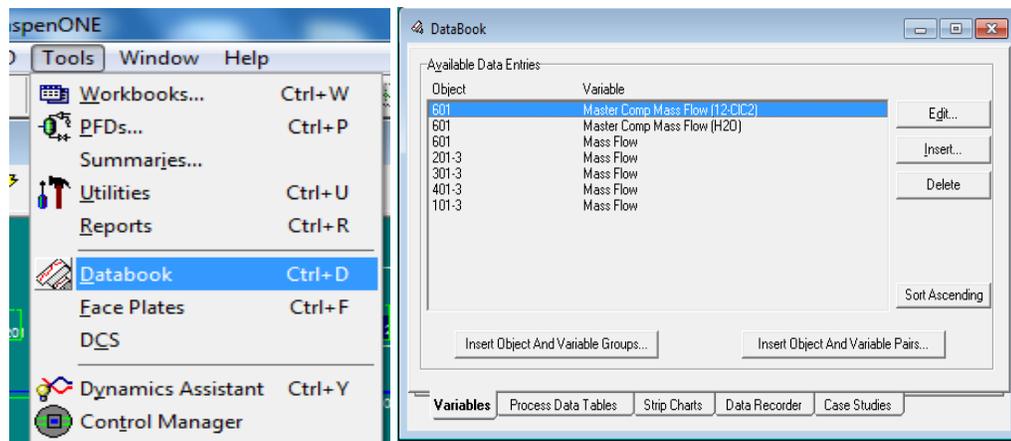


Figure 3.36: Opening databook & databook box

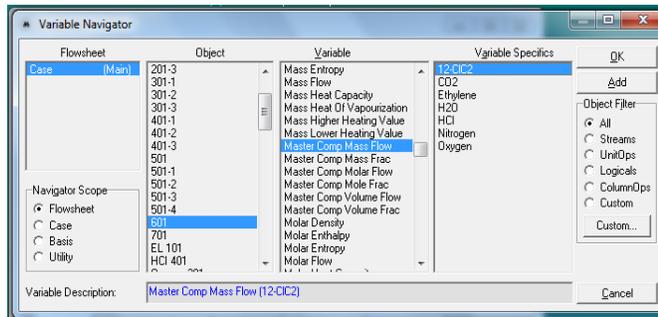


Figure 3.37: Inserting master comp mass flow

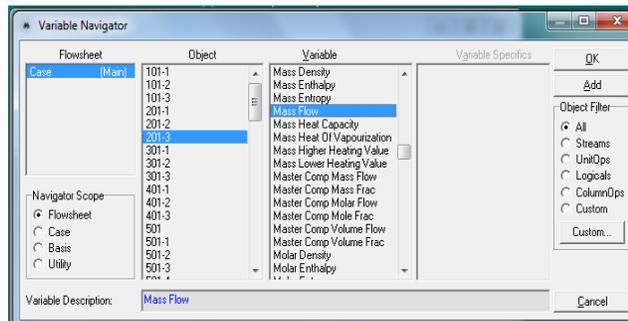


Figure 3.38: Inserting mass flow

- Click the strip chart tab. This opens the view shown in figure 3.39

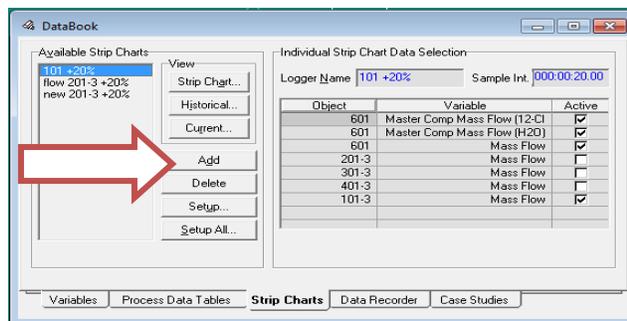


Figure 3.39: Add strip chart

7. Click Add button. This installs a data longer. You may have several strip chart
8. Specify which variables in the list on the right you want to record on this strip chart. As in figure 3.39, personnel have checked in the right column, so these four variables will be plotted on this strip chart with name strip chart that personnel want.
9. Clicking strip chart under view will bring up the strip chart window.
10. Right click on the strip chart window and select Graph Control. This opens the window shown in figure 3.40. The properties of the strip chart can be adjusted: colours, scales, label, etc.
11. If personnel is don't like the colour for background or line, only double click the background clour box in general box (figure 3.39) or colour/style/thickness at button curves on bottom tab for line (figure 3.40).

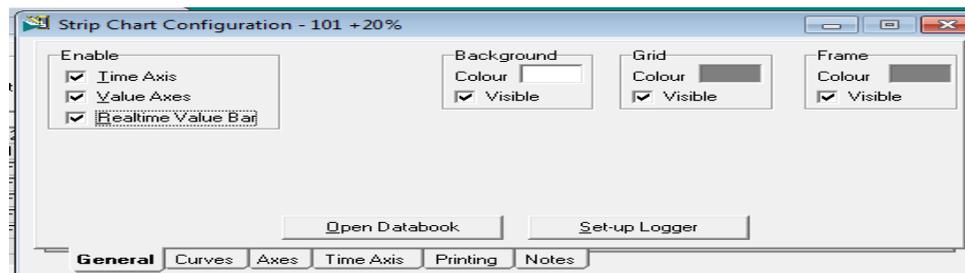


Figure 3.40: General page tab of graph control

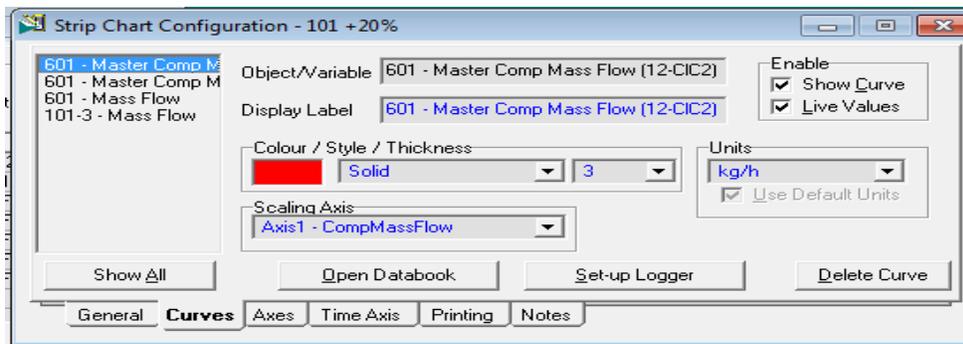


Figure 3.41: Curves Page tab of graph control

12. One important to do is to click the Set-up Logger button. The default values of the number of samples stored (300) and sampling interval (20 second) usually need to be changed to accommodate more data and more frequent sampling, particularly for the fast process.

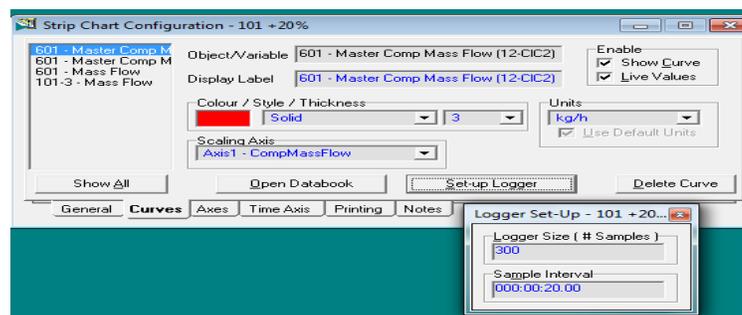


Figure 3.42: Logger setup

13. In addition to seeing the data from a dynamics run on a strip chart, these data can be saved in file and exported to some other program for plotting or analysis.

14. Go to Tools and Databook, and then open the strip chart page tab. Highlight the data logger of interest and click the historical button. A table of all the time data on the strip chart appears. The data can be saved as a file or personnel can use edit on the top tool bar to copy the data and paste them into another program.
15. By using the strip chart, personnel can define the troubleshooting in each component that involved. The overall result is in chapter 4.

## **CHAPTER 4**

### **RESULT AND DISCUSSION**

#### **4.1 INTRODUCTION**

Dynamics simulation has become increase important as processes become more complex and are designed and operated closer to constraints. Constraints are something that limited the system or process to achieve the higher performance. Increasing yields and suppressing the formation of undesirable ad environmentally unfriendly by-product are often achieved by using complex flowsheet with many recycle streams. All of these trends make dynamics control more difficult and dynamics simulation more important. It is vital that all the unit operations of complex flowsheet be able to dance together in the face of the inevitable disturbances. These include production rate changes, feed composition variability, transitions to different product specifications and rapid ambient temperature change during storms.

There are some significant steps that must be taken and vital information that must be available to go from a steady state simulation to a dynamics simulation. For this research, personnel are taking the mass flow as variable that becomes the setpoint to observe from three variables (Temperature, Pressure & Mass Flow). As is mention on the title, this research is dynamics simulation where personnel is controlling or tuning the mass flow from three streams that entering the conversion reactor to produce EDC and water in oxychlorination process. The recycle stream is addition for the ethylene stream as in recycle stream is containing more ethylene that be process back after separation section. This also help to maintain the concentration of ethylene in this process. EDC is the main product to produce vinyl chloride monomer as the purification stage. From the oxychlorination process and chlorination process, almost 95% EDC is produce. The oxychlorination become the main topic for this research because this reaction is environmentally and most waste product HCl from thermal cracking section is be used as reactant into the reactor. In addition the waste product from thermal cracking vinyl chloride monomer and purification process also is feed into the oxychlorination process. This will save the environment and avoiding the loss in cost.

In this research, personnel are controlling the flow controller where the set point (SP) becomes the manipulated variable in this process. The way to control the flow controller can be understand in chapter methodology in section dynamic simulation. The important of controlling the set point is to understand the process when personnel are needed to increasing or decreasing the mass flow of reactant. It also can be used as a first step to observe the possibility neither the process is conducted in right way or wrong. The temperature is function of conversion in this process where personnel are used conversion

reactor in this project. Therefore personnel are set up the temperature as fixed variables in this project.

As in mention in objective of research, the purpose of this research is to develop dynamics simulation of VCM process in reaction section using Aspen Hysys software. and to provide troubleshooting guideline before applied into actual plant. For the first objective, personnel has done by develop the dynamics simulation in Aspen Hysys. This step is helpful where a whole reaction section is adopted into single screen of computer. Personnel also can detect the problem occur if the process is not stabile when the steady state change to dynamics mode. For second objective, Aspen Hysys is helpful software where from the strip chart been obtained from this software is provided personnel what is trouble occur when the flow rate of reactant is increase or decrease by analysis of the transient response graph to improve the process in plant. The result steady state for each stream is like in figure 4.1.

Name	Oxygen 201	201-1	201-2	201-3	EL 101	101-1	101-2	101-3	Rec Gas 301	301-1	301-2	301-3
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature [C]	30.00	27.99	100.1	100.0	23.00	-13.80	38.17	38.14	50.00	49.78	72.65	72.60
Pressure [kPa]	1101	445.7	435.7	401.8	3251	430.0	417.1	413.9	501.3	441.7	429.6	413.9
Molar Flow [kgmole/h]	222.1	222.1	222.1	222.1	437.1	437.1	437.1	437.1	1569	1569	1569	1569
Mass Flow [kg/h]	7104	7104	7104	7104	1.227e+004	1.227e+004	1.227e+004	1.227e+004	4.630e+004	4.630e+004	4.630e+004	4.630e+004
Liquid Volume Flow [m3/h]	6.256	6.256	6.256	6.256	31.99	31.99	31.99	31.99	66.03	66.03	66.03	66.03
Heat Flow [kJ/h]	1.034e+004	1.034e+004	4.872e+005	4.872e+005	2.191e+007	2.191e+007	2.291e+007	2.291e+007	3.851e+006	3.851e+006	5.062e+006	5.062e+006
Name	501-1	501	HCl 401	401-1	401-2	401-3	501-2	501-3	501-4	601	701	*** New **
Vapour Fraction	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000
Temperature [C]	129.9	62.83	30.00	28.35	96.48	96.32	121.3	120.0	118.7	891.1	891.1	891.1
Pressure [kPa]	401.8	413.9	551.3	429.7	417.3	401.8	401.8	401.8	101.3	101.3	101.3	101.3
Molar Flow [kgmole/h]	2006	2006	885.4	885.4	885.4	885.4	2892	3114	3114	2451	0.0000	0.0000
Mass Flow [kg/h]	5.857e+004	5.857e+004	3.226e+004	3.226e+004	3.226e+004	3.226e+004	9.083e+004	9.793e+004	9.793e+004	9.793e+004	0.0000	0.0000
Liquid Volume Flow [m3/h]	98.02	98.02	37.17	37.17	37.17	37.17	135.2	141.4	141.4	108.8	0.0000	0.0000
Heat Flow [kJ/h]	3.307e+007	2.798e+007	-8.149e+007	-8.149e+007	-7.966e+007	-7.966e+007	-4.659e+007	-4.611e+007	-4.611e+007	-4.611e+007	0.0000	0.0000

**Material Streams** | Compositions | Energy Streams | Unit Ops

Fluid Pkg | All

Include Sub-Flowsheet  
 Show Name Only  
 Number of Hidden Objects

Horizontal Matrix

Figure 4.1: The result of steady state simulation.

## 4.2 TRANSIENT/ DYNAMICS RESPONSE OF EDC PRODUCT (MAIN COMPONENT) AND WATER PRODUCT (SIDE PRODUCT)

### 4.2.1 Transient/ dynamics response change in ethylene stream.

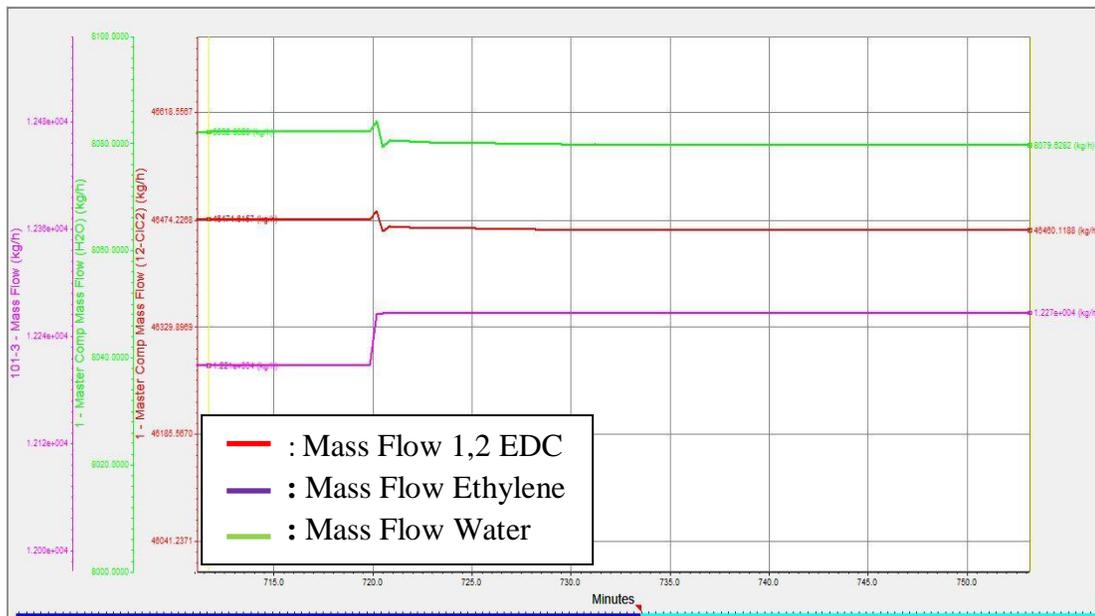


Figure 4.2: Flow rate of reactant & product (+20% of initial setpoint)

For this case of dynamics simulation, the manipulate variables is set point (SP) in ethylene flow controller where in this process, the set point is increasing as much as 20% from initial value steady state. From the observation on figure 4.2, we can conclude that the increasing the set point of flow is not helpful to increasing the main product EDC and meanwhile water is by-product. The figure above shown that the mass flow of EDC and water are decrease after the mass flows of ethylene increase when the SP increase by 20%

from initial set point. In term of reaction, the reason for the decrease the main product of oxychlorination process is the production of by-product such as 1,1,2 - trichloroethane (TCE), chloral ( $\text{CCl}_3 - \text{CHO}$ ), trichloroethylene (TRI), 1,1 - and 1,2 - dichloroethylenes, ethyl chloride, chloro - methanes (methyl - chloride, methylen - chloride, chloroform). The byproduct this is more consumes the ethylene and with steady flow of HCl and oxygen makes the main product decrease. Therefore the EDC is decrease. Second reason is the temperature feed is lower point then influent the decreasing in diffusivities of reactant in reactor. Therefore the mass transfer of EDC is decrease. Both reasons can be explore in the reaction on literature review. In the figure for the mass flow EDC and water, personnel are observing the inverse response where a few processes exhibit a behavior where for a step change in input, the output initially changes in a direction that is opposite to the final direction it will have taken when the process has fully responded to the input change. Such a process response is shown below and is characterized as an inverse response. As a physical explanation of the inverse response is a increasing the SP will affect the valve opening gives a increasing the mass flow through the valve. Although Aspen Hysys is control by computer, the valve opening also is opening by fully before this software calculates the percentages of the right percentages of valve opening. The relative velocity between the gas and liquid phases (slip velocity) in the reactor increases, resulting in reduced mass flow rate through the valve. The data for this trial can be seen on the table 4.1.

Set point (Initial): 12560kg/h

Set point (+20%): 15072kg/h

Table 4.1: Result of increasing 20% SP ethylene stream

Value	Mass Flow Ethylene (kg/h)	Mass Flow 1,2 EDC (kg/h)	Mass Flow Water (kg/h)
<b>Initial</b>	12207	46473.8	8084.964
<b>Final</b>	12270	46460.1	8079.629

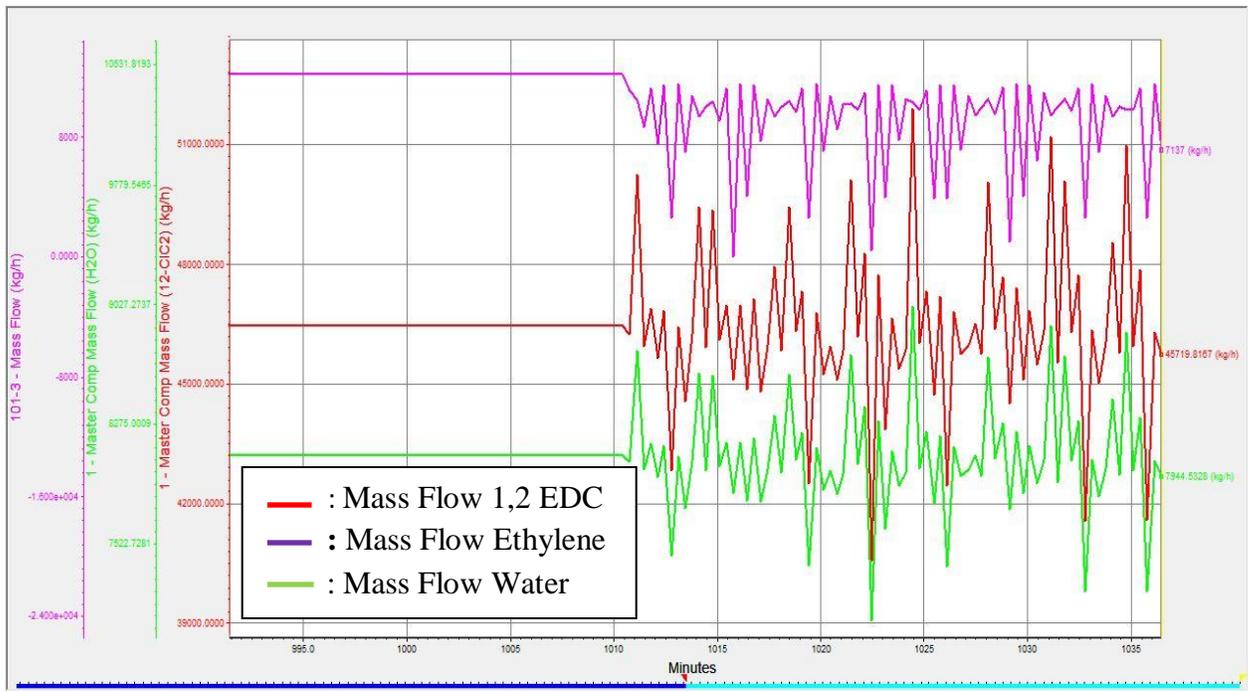


Figure 4.3: Flow rate of reactant and product (-20% of initial setpoint)

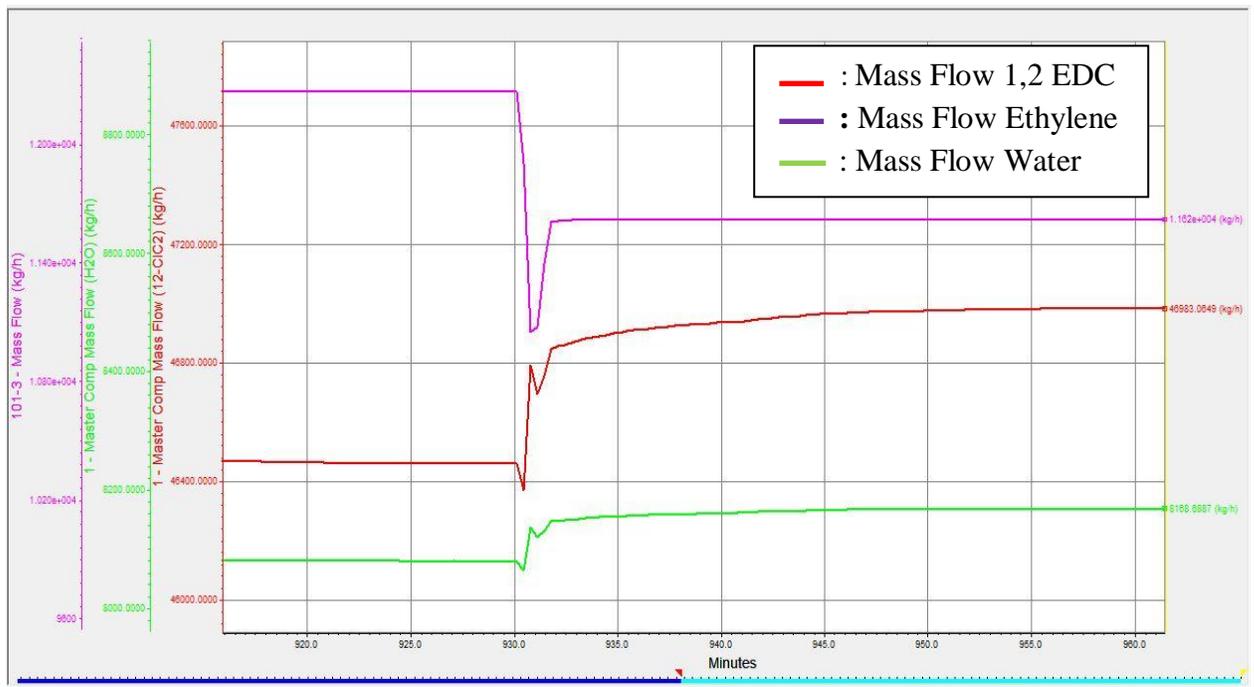


Figure 4.4: Flow rate of reactant and product (-10% of initial setpoint)

In this case of dynamics simulation, the variables be manipulate is SP of ethylene mass flow in flow controller with another stream SP is constant. For this simulation, the set point is set for decreasing of 20% from initial set point. When the set point is decrease the mass flow of ethylene, EDC and water observe from figure 4.3 is unstable. The graph is not achieved the stability in the process after a long time observation. Then personnel is test the flow controller with a new set point where for new setpoint, the SP is decreasing 10%. In figure 4.4 shows that the process is achieved stability in the system. In addition the mass flow of product is increase although the mass flow of reactant (ethylene) decreases. The reason for why decreasing 20% is unstable compare 10% is because the process is totally reject a 20% decreasing although the personnel was auto tune the flow controller into PI

and PID but the process still doesn't show any stability in the process. These conclude that by decrease the ethylene more than the limit is not a good option. In term of reaction, this is related to the slight excess of ethylene to it stoichiometric requirement in reaction. It also because the use of oxygen instead of air operation at lower temperature where this situation show the lower ethylene mass flow through the reactor giving higher production of EDC with minimal loss in overall ethylene yield. So for 10% decreasing, the process still achieved stability and increasing in product related the amount the decreasing in reactant mass flow is small. The data for this controller can be seen on the table 4.2. These graph responses also show the inverse response.

Set point (Initial): 12560 kg/h

Set point (-10%): 11304 kg/h

Set point (-20%): 10048 kg/h

Table 4.2: Result of decreasing 10% and 20% SP ethylene stream

	<b>Mass Flow Ethylene(kg/h) -20%</b>	<b>Mass Flow Ethylene(kg/h) -10%</b>	<b>Mass Flow 1,2 EDC(kg/h) -20%</b>	<b>Mass Flow 1,2 EDC(kg/h) -10%</b>	<b>Mass Flow Water (kg/h) -20%</b>	<b>Mass Flow Water (kg/h) -20%</b>
<b>Initial</b>	12207	12207	46473.8	46473.8	8084.964	8084.9
<b>Final</b>	10560	10090	unstable	46704.1	unstable	8129.3

#### 4.2.2 Transient/ dynamics response change in oxygen stream.

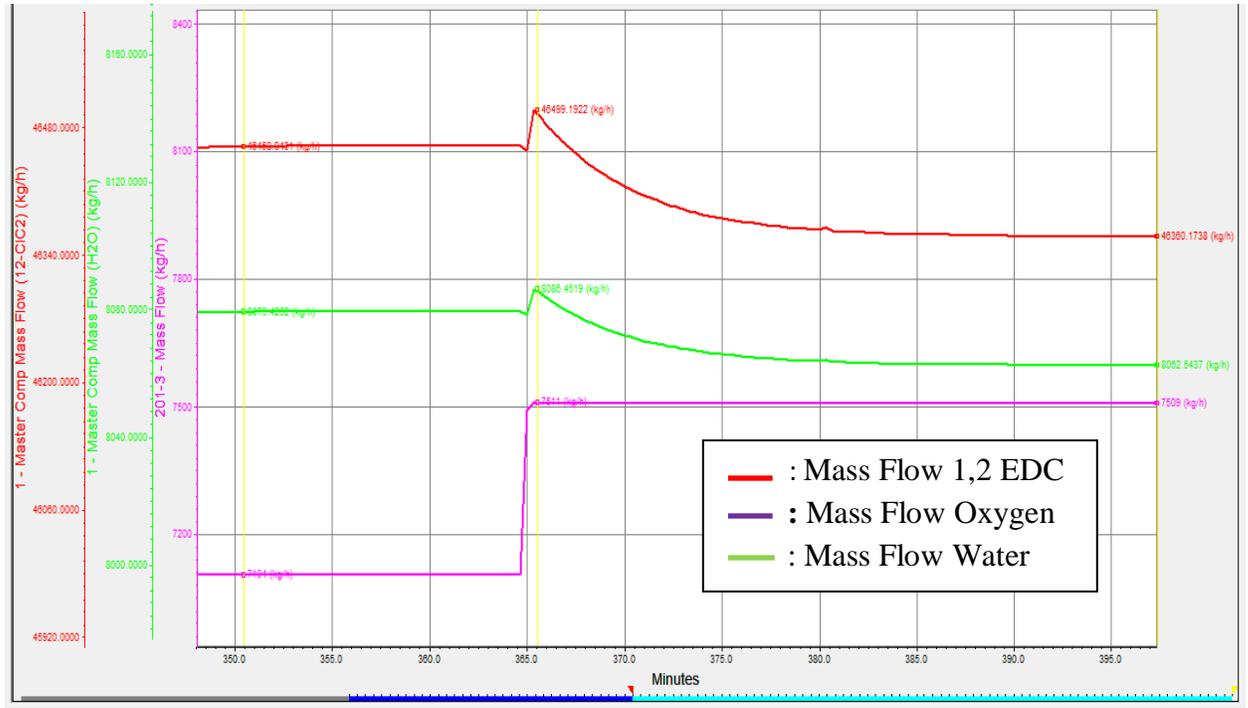


Figure 4.5: Flow rate of reactant and product (-20% of initial setpoint)

The result from this case is like in figure 4.5 where the SP of oxygen stream is manipulated by increasing 20% of initial value SP. However the result has been collected show is inversely proportional with the increasing the SP of oxygen stream. The mass flow of both products is decrease when the reactant flow increase. This has the reason for this condition. When oxygen is increase, the total ethylene lost in combustion also increase. Because of the oxygen will react with ethylene to produce more chloride gas and water vapor. Therefore the ethylene left is less to react with the hydrogen chloride to produce EDC. Also hydrogen chloride is at constant amount to react with the increasing of amount

oxygen to produce water. Moreover the reaction to produce EDC and water also has a side reaction where the 8 side reaction is produce from reaction using chloride gas and 2 side reaction using oxygen gas. In this result also personnel obtain inverse response for both flow of product. This reaction with a new SP is suppose to increase the mass flow of product but on suddenly the mass flow is drop. The reason is in this dynamics simulation, personnel are using the controller in automatic mode in parameter of controller. So the valve opening is follow the new SP by opening the valve 100% before the simulation recalculated the percentage of valve opening and mass flow is decrease until it achieved the stability.

Set point (Initial): 7104kg/h

Set point (+20%): 8524kg/h

Table 4.3: Result of increasing 20% SP oxygen stream

	<b>Mass Flow Oxygen (kg/h)</b>	<b>Mass Flow 1,2 EDC (kg/h)</b>	<b>Mass Flow Water (kg/h)</b>
<b>Initial</b>	7104	46405	8080.87
<b>Final</b>	7509	46360	8063.55

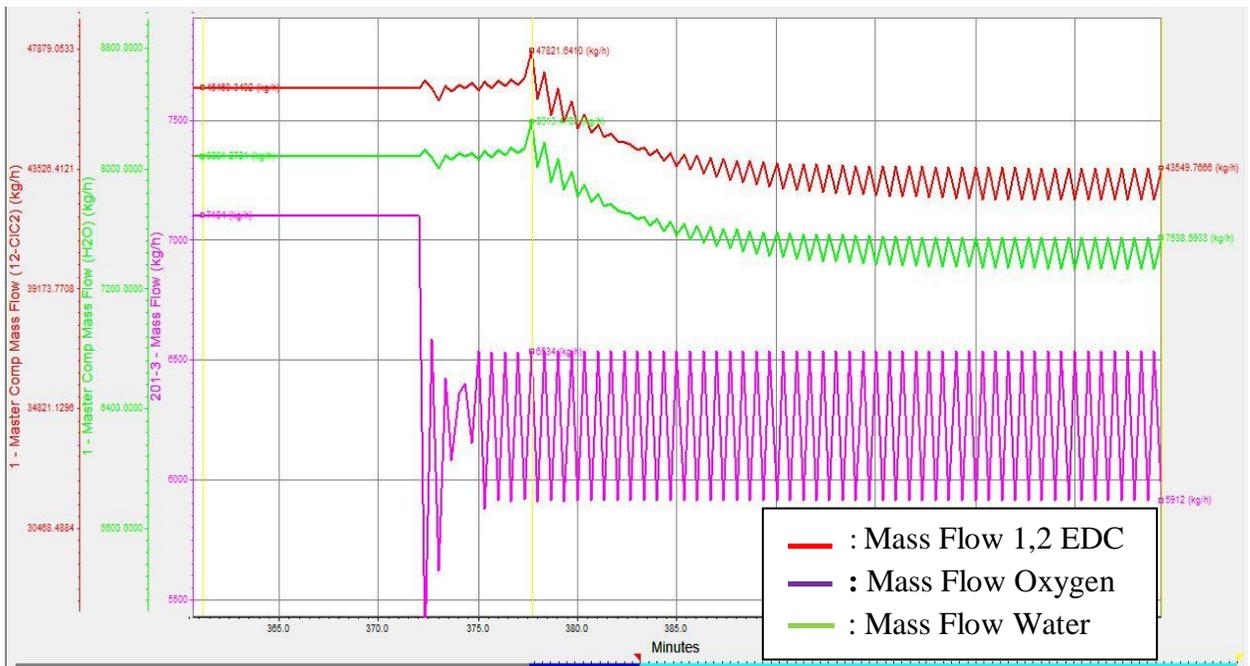


Figure 4.6: Flow rate of reactant and product (-20% of initial setpoint)

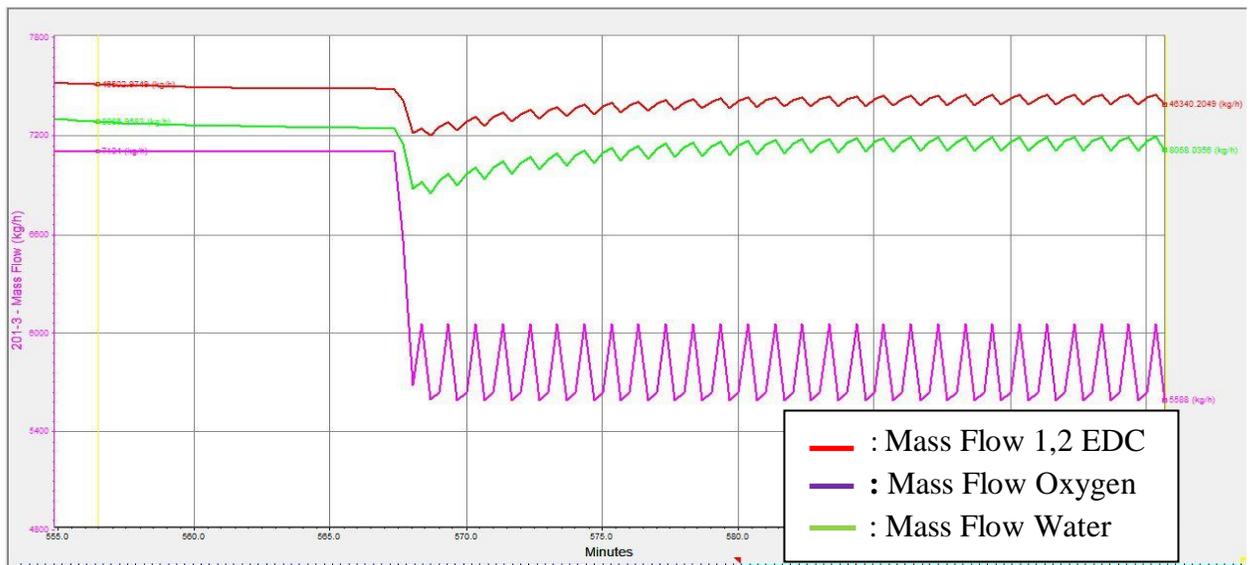


Figure 4.7: Flow rate of reactant and product (-10% of initial setpoint)

In this dynamics simulation case, the variables be manipulated variables is SP of oxygen mass flow in flow controller. The new set point is set for decreasing of 20% from initial set point. When the set point is decrease the mass flow of oxygen, EDC and water observe from graph is unstable. The graph is not achieved the stability in the process. Process is kept increase and decrease after a long time been given to the system. Then personnel are testing the flow controller with a new set point where for new SP, the SP is decreasing 10%. In figure 4.7 shows that the process also doesn't achieved stability in the system. The reason for why decreasing 20% and 10% is unstable process is because the process is totally reject set point decreasing although the personnel was autotune the flow controller into PI and PID but the process still doesn't show any stability in the process. In term of reaction, this is related to the reactions that occur in reactor. When the oxygen is decrease, the ethylene and hydrogen chlorine is unstable to find the pair to react. Therefore the reaction is chaos condition where the each reactant is not able to react with other because the oxygen is important to react with ethylene to produce chlorine gas for the main and side reaction to successfully the reaction. Such a process response is shown personnel identify that response is characterized as an inverse response. As a physical explanation of the inverse response is a increasing the SP will affect the valve opening gives a increasing the mass flow through the valve. Although Aspen Hysys is control by computer, the valve opening also is opening by fully before this software calculates the percentages of the right percentages of valve opening according the new SP. The relative velocity between the gas and liquid phases (slip velocity) in the reactor increases, resulting in reduced mass flow rate through the valve. The data and result for this controller can be seen on the table 4.4.

Set point (Initial): 7104kg/h

Set point (-20%): 5683.2kg/h

Table 4.4: Result of decreasing 20% SP oxygen stream

	Mass Flow Oxygen (kg/h)	Mass Flow 1,2 EDC (kg/h)	Mass Flow Water (kg/h)
<b>Initial</b>	7104	46405	8080.87
<b>Final</b>	5912	unstable	unstable

#### 4.2.3 Transient/ dynamics response change in hydrogen chloride stream.

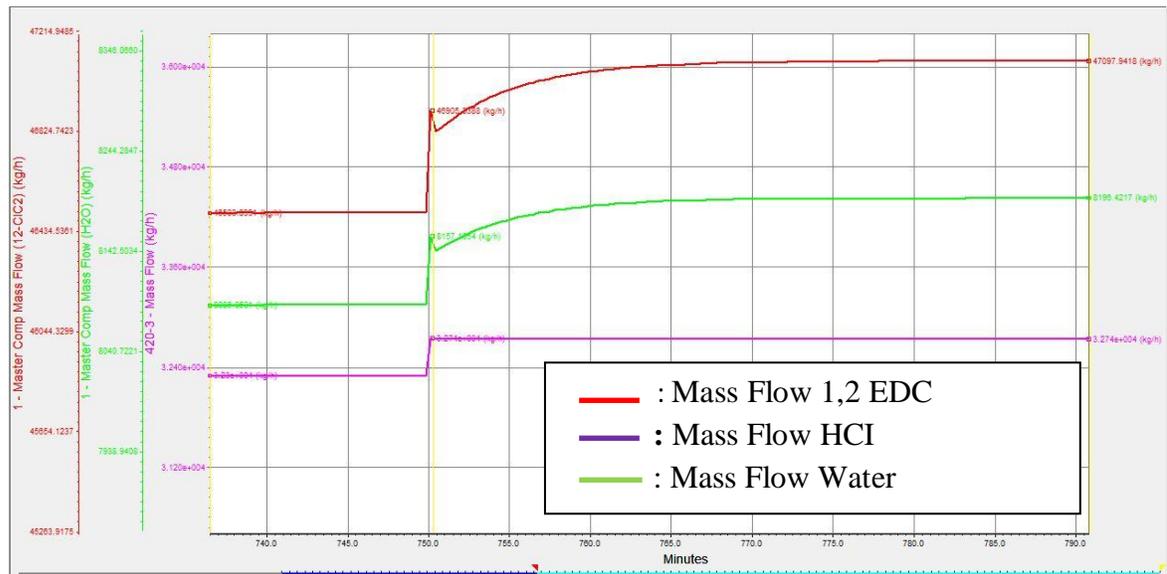


Figure 4.8: Flow rate of reactant and product (+20% of initial setpoint)

From the observation on the figure 4.8, the set point is set for increasing of 20% from initial value of SP. When the set point is increase therefore the mass flow of hydrogen chlorine is increase also. The result from this additional 20% of set point shows that the mass flow of EDC and water are increase. From the reaction, stoichiometry of hydrogen chloride is 1:1 with EDC and water. In addition, when the reaction takes place in the reactor, the mass flow of hydrogen chlorine is proportional with mass flow of product (EDC and water). The explanation that can be used to support this equation is when the hydrogen chlorine increase, the main reaction and nine more side reaction is get more enough the chlorine gas from hydrogen chlorine to react. As a mention in result before, the chlorine is useful to reaction in the reactor. With the addition hydrogen chlorine and constant mass flow of ethylene and oxygen will complete the reaction of oxychlorination reactor. From the observation the inverse response also take part in the response graph. As a physical explanation of the inverse response is a increasing the SP will affect the valve opening gives a increasing the mass flow through the valve. Although Aspen Hysys is control by computer, the valve opening also is opening by fully before this software calculates the percentages of the right percentages of valve opening. The data for this trial can be seen on the table 4.5.

Set point (Initial): 29550kg/h

Set point (+20%): 35460kg/h

Table 4.5: Result of increasing 20% SP hydrogen chloride stream

	Mass Flow Hydrogen Chloride (kg/h)	Mass Flow 1,2 EDC (kg/h)	Mass Flow Water (kg/h)
<b>Initial</b>	32295	46509	8087.92
<b>Final</b>	32740	47097	8196.42

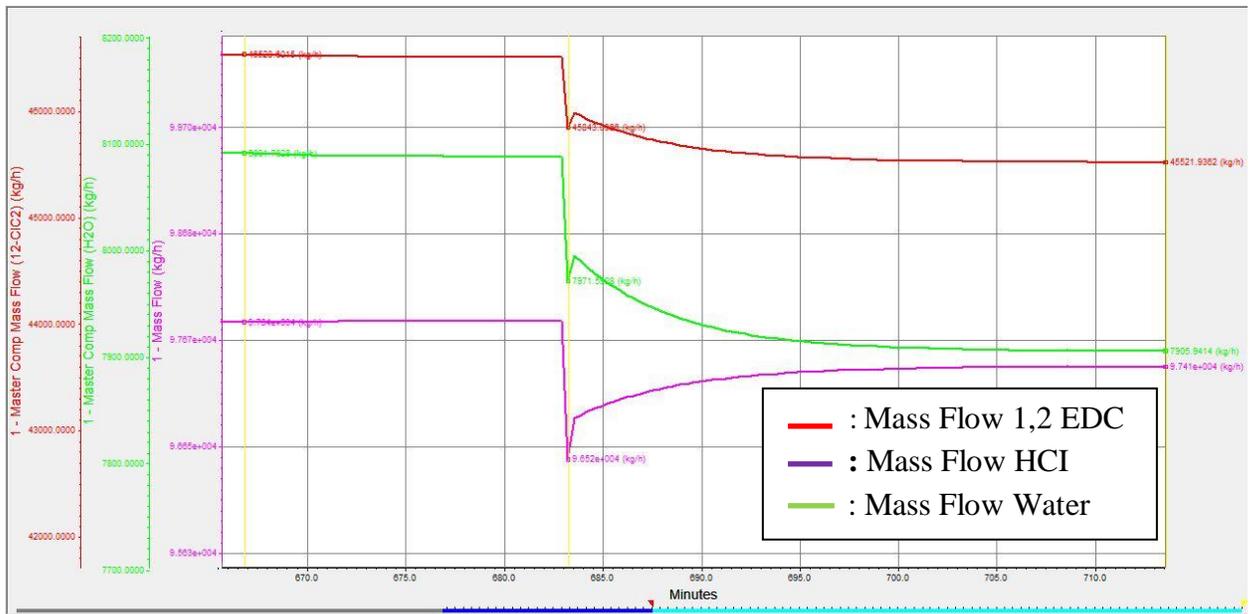


Figure 4.9: Mass flow of reactant and product (-20% of initial setpoint)

In this dynamics simulation for new set point (SP) in flow controller of hydrogen chlorine, personnel is detect that the EDC and water mass flow is decrease along the mass flow of hydrogen chloride when the SP is change by decreasing 20% from initial SP value. This situation is vice versa than situation in increasing SP for same stream. In this

simulation the SP of flow controller is set decreasing 20% to obtain the effect of this stream to production of product. As personnel can see from figure 4.9, the product is decrease along the reactant. Personnel also can detect inverse response in three line of mass flow. These conditions occur when the controller is set in automatic mode. When personnel change the SP on suddenly action, the valve opening is also involve where Hysys simulation will automatic control the opening of valve until the stabile calculated mass flow of hydrogen chlorine achieved. In term of reaction, this process is show that the hydrogen chlorine is important raw material because among all the reaction including side reaction are using hydrogen chlorine as the reactant. The data for this trial can be seen on the table 4.6.

Set point (Initial): 29550kg/h

Set point (+20%): 23640kg/h

Table 4.6: Result of decreasing 20% SP hydrogen chloride stream

	<b>Mass Flow Hydrogen Chloride (kg/h)</b>	<b>Mass Flow 1,2 EDC (kg/h)</b>	<b>Mass Flow Water (kg/h)</b>
<b>Initial</b>	32295	46509	8087.92
<b>Final</b>	31550	45521	7905.94

## **CHAPTER 5**

### **CONCLUSION & RECOMMENDATION**

#### **5.1 CONCLUSION**

The VCM case study emphasizes the complexity of designing a large chemical plant with an intricate structure due to reactors and separation sections. In this research the oxychlorination is taking place as an important process based on the relevant this process to environment, society and management. These processes are sources of the intermediate EDC, which is a reactant in the pyrolysis to produce vinyl chloride monomer. From the observations in chapter 4 result and discussion, personnel have identify that some manipulate variable will affect the production either the give high production or low production when the value of SP is changed. In this research, personnel identify that the production of EDC increase when the mass flow of ethylene and mass flow of HCl increase. The streams that make the production of EDC decrease is when the mass flow of

ethylene, oxygen increase with addition the mass flow HCl stream decrease. The unstable of reaction occur when the mass flow oxygen decrease. So the mass flow of oxygen stream is needed to take more serious because this stream is one factor in exothermic reaction that these processes undergo. As conclusion, this research is fulfill the objective of research and highly beneficial and most helpful researcher for industries to analysis any question or problems that related to abnormal of process production VCM in reactor section using dynamics simulation to obtain quality and quantities product before start applied into real plant.

## **5.2 RECOMMENDATION FOR FUTURE RESEARCH**

The recommendation for this research is these researches can be continues by other personnel including separation and purification VCM section. It will be completed a whole VCM plant in single screen. Therefore the VCM plant will working in high efficiency process where all the problem that in future will happen in this process will been prevented first and the troubleshooting procedure will be prepare for future to ensure these process appear as green process that take care for environment, society and human life.

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# APPENDIX A1

## Full steady state with controller flowsheet

