DEVELOPMENT OF OPERATOR TRAINING SIMULATOR USING ASPEN SIMULATION WORKBOOK (ASW): A REACTOR CASE STUDY

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DEVELOPMENT OF OPERATOR TRAINING SIMULATOR USING ASPEN SIMULATION WORKBOOK (ASW): A REACTOR CASE STUDY

FARAH SYAHIRAH BINTI YAHYA

Thesis submitted in partial fulfilment of the requirements
for the award of the degree of
Bachelor of Chemical Engineering

Faculty of Chemical & Natural Resources Engineering
UNIVERSITI MALAYSIA PAHANG

JUNE 2015

SUPERVISOR’S DECLARATION

We hereby declare that we have checked this thesis and in our opinion, this thesis is adequate in terms of scope and quality for the award of the degree of Bachelor of Chemical Engineering.

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Date	: JUNE 2015

STUDENT'S DECLARATION

I hereby declare that the work in this thesis is my own except for quotations and summaries which have been duly acknowledged. The thesis has not been accepted for any degree and is not concurrently submitted for award of other degree.

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DEDICATION

This thesis is dedicated to my family and friends. A special feeling of gratitude to my loving parents, a strong and gentle soul whose taught me to trust in Allah, believe in hard work and that too much could be done with less. My siblings, for their words of encouragement and a push for tenacity ringing in my ears.

I also dedicate this thesis to my friends who have supported me throughout the process. I will always appreciate all they have done, for supporting me to believe in myself.

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ABSTRACT

Operating Training Simulator (OTS) is a computer-based training system. The OTS applies a simulation of an industrial process to generate the appropriate data of the plant's process operation. In addition, the OTS is widely accepted in the industry as an enabling technology for employee competency and proficiency training and enhancement. This system is deemed as the effective application in order to develop the highest skill levels and proficiency of the operator. This project presents the first-hand experience of developing a process simulator system using Aspen Simulation Workbook (ASW). The production of acetic acid from methanol carbonylation is used as a case study. Aspen Plus is used for the modelling of the methanol carbonylation process and will be linked with Excel using Aspen Simulation Workbook. The simulation can be operated in Aspen Simulation Workbook by manipulating the value of the variables. This case study is about to determine the changes of output variable by manipulates the input variables. This would contribute towards the solution of training issues related to control and operate a process and act as a tool to educate and train the engineering students for supporting training in control and operate certain processes respectively. The operator training tool is developed successfully in Aspen Simulation Workbook.

ABSTRAK

Operasi Simulator (OTS) merupakan satu sistem latihan yang berasaskan komputer. OTS telah mengaplikasikan proses simulasi perindustrian untuk menghasilkan data yang sesuai bagi operasi proses sesebuah kilang. Disamping itu, OTS telah diterima pakai secara meluas dalam industri sebagai satu teknologi yang boleh meningkatkan kecekapan dan latihan kemahiran untuk para pekerja dan kecekapan operator. Sistem ini disifatkan sebagai satu aplikasi yang berkesan dalam usaha untuk membangunkan tahap kemahiran tertinggi dan kemahiran pengendali. Kertas kerja ini membentangkan pengalaman dalam membagunkan proses simulator sistem, dengan menggunakan Aspen Simulasi Buku Kerja (ASW) untuk pengeluaran asid asetik dari methanol carbonylation. Aspen Plus dan dinamik digunakan untuk membangunkan model reaktor yang berkeadaan tetap bagi menghubungkan dengan Microsoft Excel menggunakan Aspen Simulasi Buku Kerja. Ini akan menyediakan integrasi lancar antara model simulasi proses Aspen Tech dan alat kejuruteraan lain dengan lembaran kerja Microsoft Excel tanpa memerlukan pengaturcaraan dan ini juga memudahkan pengguna lain yang tiada pengalaman berkaitan proses simulasi memanipulasi Simulasi Aspen Plus yang kompleks dari Excel. Simulasi ini boleh beroperasi dalam Aspen Simulasi Buku Kerja dengan memanipulasi nilai pembolehubah. Kajian ini adalah untuk menentukan perubahan output berubah dengan memanipulasi pembolehubah input. Ini akan menyumbang kepada penyelesaian isu-isu yang berkaitan dengan latihan mengawal dan mengendalikan proses dan bertindak sebagai alat untuk mendidik dan melatih pelajar-pelajar kejuruteraan untuk menyokong latihan dalam mengawal dan mengendalikan proses tertentu masing-masing. Alat latihan pengendali dibangunkan dengan jayanya di Aspen Simulasi Buku Kerja..

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LIST OF ABBREVIATIONS

OTS	Operator Training Simulator
ASW	Aspen Simulation Workbook
SHE	Process Safety, Health and Environmental
APC	Advance Process Control
CAPD	Computer-aided process design
UK	United Kingdom
USA	United State of America
DCU	Delayed Coker Unit
T	Temperature
P	Pressure
CH_3COOH	Acetic Acid
H_2O	Water
CO	Carbon Monoxide
CH_3OH	Methanol
CO_2	Carbon Dioxide
H_2	Hydrogen
GUI	Graphic User Interface

1 INTRODUCTION

1.1 Motivation and statement of problem

Correct and efficient process operation is becoming increasingly important in the chemical industry as safety requirements and environmental specifications are getting stricter (A.L.Ahmad et al., 2010). 'Safety First' is a tagline that commonly found in almost workplace throughout the world. A numbers of safety policies and standardizations are in place to govern the compliance of safety practice in the workplace (Preston et al.,, 1996). It is well recognized and accepted that safety issue is the most important aspect of industry process operations (Ming et al.,, 2003). Basically, the competency of the operator is really essential to guarantee safety in a workplace. Thus, current employee and operators continually seeks way to improve and increase the competency and performance of its workforce since many workplaces especially chemical plants become more automated (A.L.Ahmad et al., 2010).

The technological development during the last ten years has made simulators for training the engineers and operators in receiving hands-on training ahead of the plant operation, and due to this purpose OTS is considered a necessity in the development of the entire industry (ION, 2010). Adoption of training simulators has been widely practiced in industries where capital investment is high, processes with high complexities and enormous hazardous consequences in case of failure and the industries are not limited to chemical processes, but are also apparent in aviation, shipping, power and energy industry, medical and nuclear system (Cameron et al., 2002, Yang et al., 2001, Murugappan, 2009, Merritt, 2006, Seccombe, 2008).

In the chemical industry, especially in the case of processes, operator training simulators (OTS) are becoming widely used. Operating training simulators (OTS) are computer-based training system for developing and maintaining operational skills in a variety of technical systems (Mani et al.,1990; Kobashi et al., 1995; Okapuu-von Veh et al.,1996; Dudley et al.,2008; Balaton et al., 2013; Manca et al.,2013). With the help of these systems several operations and safety issues can be analyzed, and the operating staff of the plant can be trained in handling different plant failures (Fürcht, Kovács, & Rabi, 2008; Rey, Thiabaud, & Tourdjman, 2008; Yang, Yang, & He, 2001).

Recently, many chemical companies have decided to use OTS system as a tool for training operating staff, rarely used modes of operation and measuring their skills, as well as supporting engineering tasks like testing new methods and performing safety test without risk on the real system. To fully accomplish the OTS successfully, a structured model of high computational complexity comprising a large number of state variables and parameters. Several often difficult to measure or determine, is required. However, for computational reasons the OTS model should preferably be kept as simple as possible. The main part of the OTS is the process model that replaces the real technology and an OTS is an example of high fidelity simulation model application. These models are mathematical representations of actual plants that accurately mimic the process conditions on the plant using chemical engineering theory (Jago, 2008).

Training, or person's readiness, is perhaps the most important aspect of the success of operational readiness. An untrained operator is not competent to run the plant to the optimum degree of efficiency. Taking an analogy to autopilot, advanced process control (APC) typically removes the reactive actions required by a process operator to allow more time to be spent on optimizing production. However, from time to time, operators need to be able to take control of the process to manage an upset. This gap can be filled by an OTS, analogous to a flight simulator, it is proved to be extremely valuable, allowing the operator to continually develop skills, make mistakes and learn in a safe simulated environment (ARC, 2009, Merritt, 2006, Murugappan, 2009). For ensuring the effectiveness of an OTS, its backbone, the models need to be rigorous and robust enough to cover all the operations. These high fidelity models need to represent key operating scenarios such as start-up, shutdown, normal operations and also abnormal situations, such as equipment failure (Mhammed, 2005) (Muravyev A. a., 2007). This feature is inarguably the most important and vital element for a good and reliable simulator.

OTS system also can be used in an educational sector as a tool to educate and train the operators for supporting training in control and operate certain processes. Pre-training in the OTS environment prior to practical training in the plant or laboratory environment could significantly enhance the efficiency of learning of the process operators. In particular, the operators' understanding of the complexity of the process, ability to make correct operational decision and adhere to standard routines could be expected to be improved (Lee, 2005). So far, few efforts have been made to exploit the potential of OTS for supporting training in process manufacturing. Especially, production processes may benefit substantially by using OST due to their inherent complexity, complicated operational procedures and wide-spread use in large-scale industrial production.

Computer-aided process design (CAPD) and simulation tools have been successfully used in industries since the early 1960s for the development and optimization systems. Simulators used in these industries are designed to simulate processes and their behavior, mainly for process control purposes. From the available simulators, Aspen Plus (Aspen Technology,Inc.), HYSYS (Aspen Technology,Inc),and PRO/II (Simulation Sciences,INC.) are the most widely used. In OTS applications, the entire plant is to be simulated. However, the simulation of the auxiliary units might be more difficult. The most advantageous solution would be the connection of these software programs. Numerous studies have been conducted to elucidate the functions and benefits of operator training simulator (OTS) in the industry. Although the function of OTS is well understood, however, no research has been performed for developing an operator training simulator by using Aspen Simulation Workbook (ASW), and therefore this is the aim of this study.

ASW enable seamless interoperability between AspenTech's engineering tools and Microsoft Excel with no programming required. ASW is a powerful tool that allows Aspen Plus and Aspen HYSIS simulation experts to easily create a clean user interface for their models in Microsoft Excel. This makes it easy for other users to manipulate complex Aspen Plus simulations without being intimately familiar with the models or even the software used. It brings the power of process modelling to a wider range of users, allowing us to expand the use of process models to solve plant operating problems (Aspen Technology,Inc, 2014). The main objective of this study was to develop operator training simulator using Aspen Simulation workbook for reactor case study and the production of Acetic acid via methanol carbonylation process was chosen as a case study for this project.

1.2 Objectives

The following are the objective of this research:

- To develop an operator training simulator by using Aspen Simulation Workbook (ASW) for a production of acetic acid process.

1.3 Scope of this research

The following are the scope of this research:

i) **Develop a reactor model** to produce acetic acid via a methanol carbonylation process by using Aspen PLUS.

ii) **Develop GUI and Embedding the simulation** case files using Aspen Simulation Workbook (ASW) in Microsoft Excel.

iii) **Test the Operator Training Simulator (OTS)** by running scenarios of case study.

1.4 Main contribution of this work

The following are the contributions

i) Solution of training issues related to control and operate a chemical process.

ii) Tools to educate and train the engineering students or inexperienced operators for supporting training in control system changes and test those changes against the simulator.

1.5 Organisation of this thesis

The structure of the reminder of the thesis is outlined as follow:

Chapter 2 provides a summary of the literature of Operator Training Simulator (OTS) in worldwide company and the previous work on the production of acetic acid process by methanol carbonylation. General descriptions of the flow characteristic of the system, as well as the information on reaction are presented. This chapter also provides a brief description of the reactor operating conditions, including the type of the reactor, the temperature, and also the pressure of the reactor used. A brief description of the simulation software is also provided.

Chapter 3 gives a review of the methodology for the development of Operator Training Simulator using Aspen Simulation Workbook for acetic acid production. This chapter discuss on the developing simulation model by using Aspen Plus and also the steps to connect the simulation model with the Excel by using Aspen Simulation Workbook.

Chapter 4 discuss about the result of the case study of acetic acid production. The model is developed using Aspen Plus simulation software based on the data from previous kinetic modelling. The reactants used are methanol, carbon monoxide and water and the main product of the process is acetic acid.

Chapter 5 is about the conclusion from the objectives of the experiment and some recommendations to improve our skills in simulator training.

2 LITERATURE REVIEW

2.1 Overview

This paper presents the development of Operator Training Simulator (OTS) using Aspen Simulation Workbook for the production of Acetic Acid by methanol carbonylation case study. The technological development during the last ten years has produced simulators as a tool for training engineers and operators in receiving realistic hand-on training ahead of the plant start-up and throughout plant operation. Due to this purpose, the simulator has been considered a necessity in the development of the entire industry since correct and efficient process operation becoming increasingly important in the chemical industry as safety requirements and environmental specification is getting stricter. The simulation model was done using Aspen Plus. Then, the integration between the simulation model with Microsoft Excel is provided by Aspen Simulation Workbook (ASW). Then, the ASW will allow modelling experts to link model and plant data and publish the resulting model as Excel worksheet.

2.2 Recent Development of Operator Training System in Industry

The first Operator Training System was developed and launched in MOL's Danube Refinery at Százhalombatta in the Delayed Coker Unit (DCU), paralelly to unit start-up in 2001. The advanced technical state of the Danube Refinery and the further developments generated extended demand for skilled and well-educated employees. In order to meet this demand, the Refinery management decided to upgrade the existing OTS in the Delayed Coker unit and to implement new systems for the most important units. After the project definition period the OTS Project started at the Danube Refinery in 2005. Based on the results further steps are planned: more Training Systems will be implemented in the 2007-2010 timeframe. (ákos Fürcht, kovács, & rabi, 2008).

The purpose of simulations is that by simulating a process the engineers can follow and view the entire system over time, without having to change, interrupt and affect it. It is important to remember that the decision they make and the actions they take can have a deep impact on the project success indicators involving areas related to cost, risk, quality and schedule. The dynamics of complex processes are not exact replicas of the real system dynamics, but it is an approximation that makes the relationships between different parts of the system possible to understand (Ferreira et al., 2012). On the market today there are different tools available for both dynamic and steady state simulations. Ideally, it should be easy to switch between the two simulations and therefore it is important that the two models can be simulated in the same tool without changing the environment. In order to include both experienced and non-experienced engineers and operators, it is important that the simulator is easy to use (Bezzo et al., 2004).

In the chemical field, KBR has an outstanding team of technology, simulation and training experts who help translate our business goals of safe, economic and reliable operation into tailored solutions for our facility. The KBR, Inc (Kellog Brown & Root) are an American engineering, construction and private military contracting company which is a worldwide company that include the Americas, Africa, Asia-Pacific, Australia, Europe and the Middle East .(KBR, 2013)

An Operator Training Tool System (OTS) is the only tool that ensures plant operators receive plant specific and realistic hands-on training ahead of plant start-up and throughout plant operation. KBR's user-friendly OTS systems are configured with KBR’s proprietary reactor models and physical property methods and include scenarios that are particular to our specific plant and process. As a complement to classroom training, a comprehensive portfolio of training scenarios allows operators to reach competency in a safe, realistic, repeatable and hands-on environment. (KBR, 2013)

Benefits of OTS Include:

i. A typical 30% reduction in the training time of an experienced workforce
ii. For a non-experienced workforce, training times drop from one-three years to six months
iii. A three-five day reduction in the initial start-up time of a typical process plant
iv. Confidence knowing that plant automation systems are fully tested prior to start up

Long Term Benefits of OTS Include:

i. Operational best practices are reinforced through refresher training
ii. Increases workforce flexibility through cross-trained operators
iii. The opportunity to test trial modifications to the plant's control and automation systems and process configurations
iv. The development and refinement of operating procedures
v. OTS training helps accelerate Advanced Process Controls (APC) implementation

KBR enhance the value of OTS systems by deploying integrated engineering, commissioning and simulator teams on projects. In this way the user is able to drive synergies between and across projects that deliver increased benefits to our customers. (KBR, 2013)

2.3 Feature of an Operator Training Simulator

This OTS is used for training in both the process behavior of the plant as well as the use of distributed control system (DCS) to control the plant. As actual hardware of a DCS is very costly, a very good emulation of DCS graphics and control outlook was adopted. Figure 2-1 shows the analogy of OTS to real plant. The plant dynamic model and the actual process plant were analogous. The instructor station could be considered an analogy to the control system in real plant, where it invokes responses from operator through the operator control console. The operator console or DCS of actual plant is analogous to the emulated operator consoles.

Besides training for plant start-up, shutdown and normal operation, OTS training also covers emergency situation handling. Through instructor station, various possible condition could be initiated. A few examples were the cold start up, hot startup, emergency shutdown and malfunctions such as pump tripping.

Training would be more meaningful and effective if evaluation could be carried out. Hence, OTS does include evaluation function for tracking of operating procedures and actions in order to measure a trainee's performance. The instructor could define the acceptable operating ranges and specified a time frame for process recovery as the basis for the evaluation.

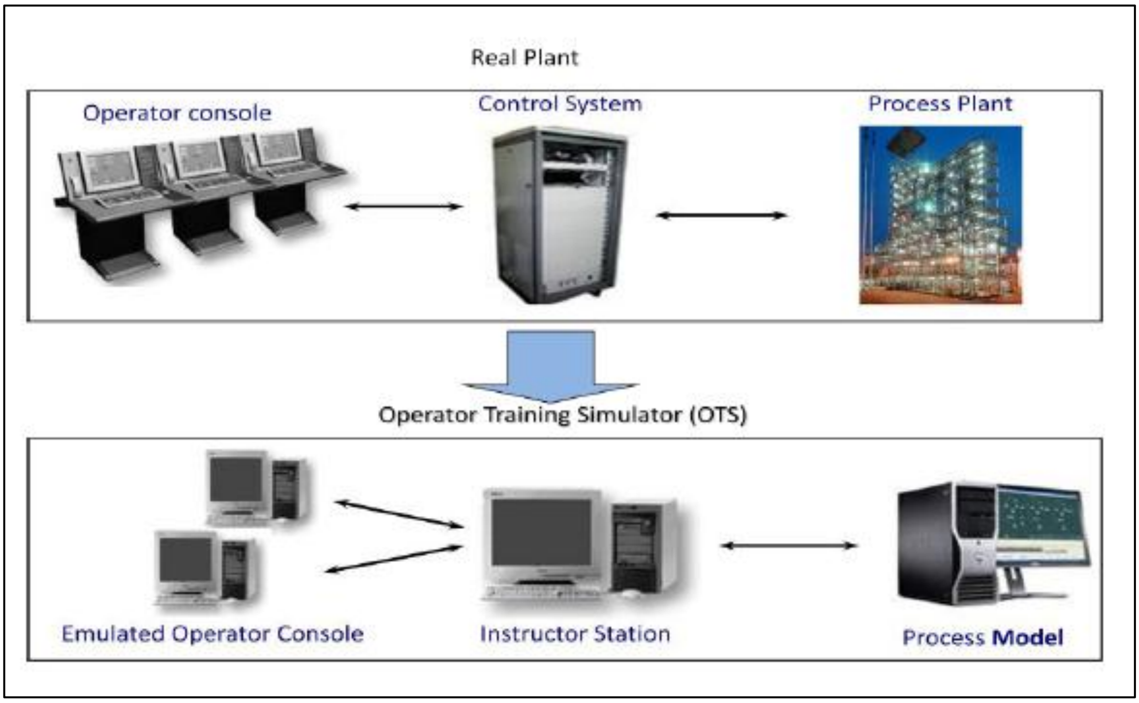

Figure 0-1: Operator Training Simulator System in Industry

The Figure 2-1 was showed the operator training simulator system in industry which is OTS solution is a cost effective high-fidelity simulated operator training solution that realistically resembles the operator station appearance and functionality, while at the same time, increases the training capabilities and flexibility of the system. The OTS will offer a highly realistic representation of plant operation and will provide a unique environment for developing operation skills and studying detailed process behaviour, using customized simulation models. Various operational conditions will be provided for the simulated plant, including start-up, shutdown, emergency conditions and normal operational transients.

2.4 Previous work on Production of Acetic Acid from Methanol Carbonylation

Acetic acid has been very familiar to mankind since it has been used as vinegar for a long time and the demand of acetic acid is about 5.4 million tons/year in the world in 1997. Acetic acid is used in vinyl acetate, solvent for the production of pure terephthalic acid (PTA), acetic anhydride, acetates, and others. In the mean time, the manufacturing process of acetic acid by the carbonylation of methanol was developed. This process uses methanol and carbon monoxide as raw materials which are produced from natural gas, coal, heavy residual oil, and others. BASF (Germany) industrialized this process in 1960, and Monsanto (USA) industrialized it in 1970. Especially the latter process, known as Monsanto process, has become the dominant industrial route for acetic acid manufacturing.

This methanol carbonylation, which is also called as Monsanto process, uses methanol and carbon monoxide as the raw materials to synthesize acetic acid. Because the price of naphtha has risen and the relatively cheap methanol, produced from off gas, natural gas, and so on, has been available after the oil crisis, this process has rapidly become prevalent. At present, this process accounts for 60% of the production capacity of the world. The overall stoichiometry of the acetic acid synthesis is represented simply by

$$CH3OH + CO \rightarrow CH3COOH$$

In the Monsanto process, the selectivities to acetic acid based on methanol and carbon monoxide are 99% and 90%, respectively, when rhodium is used as a catalyst and iodine as an activator. These days, most of the methanol carbonylation process has adopted this catalyst system (Ken-ichi Sano., Hiroshi Uchida., Syoichiru Wakabashi, 1999).

The flowsheet of methanol carbonylation process was shown in Figure 2-2. Methanol and carbon monoxide are supplied continuously into the reactor. The exhaust gas from the reaction section, together with exhaust gas from the purification section, is washed in the scrubber, then the light-ends are recovered and recycled to the reaction section. On the other hand, the reaction product (crude acetic acid) is sent to the light-ends column, and acetic acid is taken out as a side-cut. The overhead and the bottoms including the catalyst return to the reaction section. Side-cut acetic acid is sent to the dehydration column, then the mixture of water and acetic acid is taken out from the top, and returned to the reaction section. The bottoms of the dehydration column are sent to the subsequent product column. A small amount of the heavy-ends,which contain propionic acid, is taken out from its bottom.The overhead is further purified in the next fractionation column, and purified acetic acid is obtained as a side-cut.The overhead and the bottoms of the fractionation column are recycled into the reaction section.

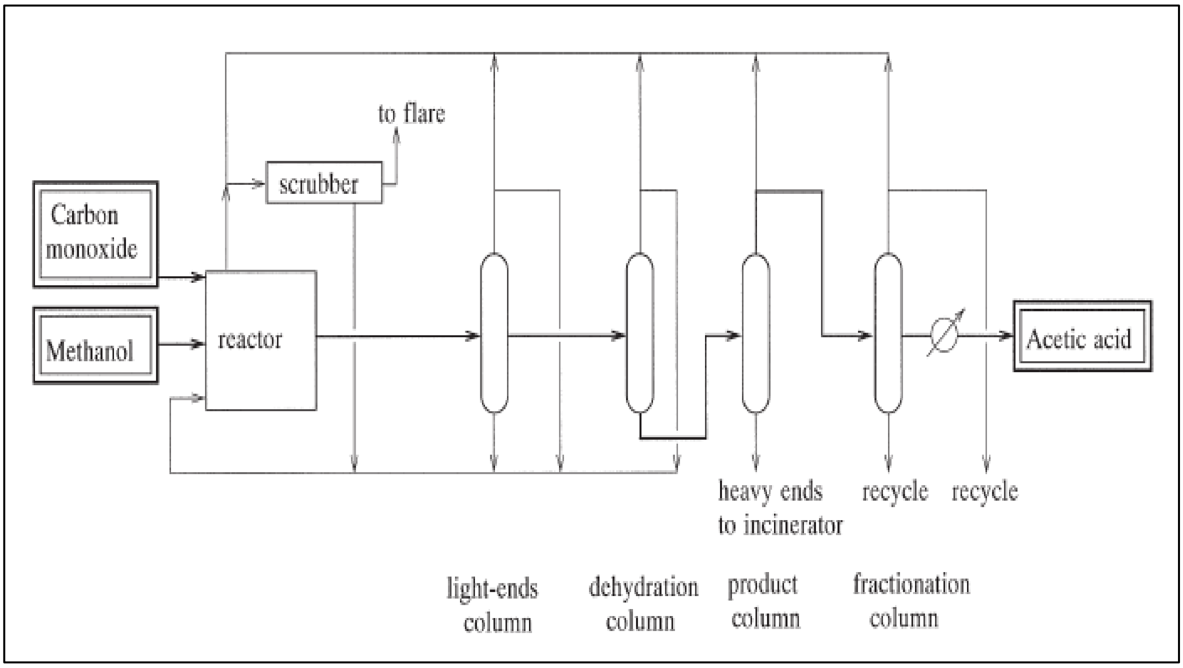

Figure 0-2: Process flowsheet of methanol carbonylation process

2.5 Simulation for develop model

In this research, the software that were used to develop an operator training tools is Aspen Simulation Workbook whereas the steady-state simulation was done using Aspen Plus. Aspen Plus is a comprehensive chemical process modelling system, used by the world's leading chemical and specialty chemical organizations, and related industry to design and improve their process plants. In addition, Aspen Plus also takes a steady - state process modelling to the next level, allowing to create powerful dynamic simulation for better analysis of plant behavior and safety.

Aspen Simulation Workbook is one of the sub-programme from the AspenTech. Aspen Simulation Workbook enables integration between AspenTech's simulators, such as Aspen Plus and Aspen HYSYS, and Microsoft Excel. For plant operations, Aspen Simulation Workbook accelerates the adoption of process models for operations decision support, bringing the power of simulation to non-simulation experts (Aspen Technology, 2004).

Aspen Simulation Workbook (ASW) is a tool for interfacing AspenTech's process simulation models with Microsoft Excel worksheets. Aspen Simulation Workbook also has tools to link model variables to plant data tags imported using third-party applications. These capabilities allow modelling experts to link models and plant data and publish the resulting models as Excel worksheets for use by casual model users(Aspen Technology, 2004).

2.6 Summary

This paper presents how an Operator Training Simulator (OTS) works in industry. Nowadays, the companies would like to operate the plant using systems because they know the benefits from the technology will contribute more to the company. Instead of the system is low cost, it also care for environment surrounding to improve safety and increase their overall profitability, always cognizant of environmental impact.

3 SIMULATION METHODOLOGY

3.1 Overview

This paper presents the development of Operator Training Simulator (OTS) by using Aspen Simulation Workbook (ASW) and solve the problem of the reactor case study . ASW provides seamless integration between AspenTech's engineering tools and Microsoft Excel, allowing us to deploy models to a wider range of users. The result is new levels of value to improve productivity during conceptual design and the expanded use of process models in operations for performance monitoring, better decisions, and optimization. Therefore, ASW is a powerful tool for creating convenient user interfaces to Aspen Plus model in Microsoft Excel. It brings the power of process modeling to a wider range of users, allowing us to expand the use of process models to solve plant operating problems such as equipment troubleshooting, performance improvement and other plant studies, driving greater value from my simulation investment. This makes it easy for other users without process simulation experiences to manipulate complex Aspen Plus simulation from Excel (Leviene & Tremblay, 2012). In this study, the reactor model was designed and developed by using Aspen Plus. Then, the graphic user interface (GUI) of the OTS was developed and embedded in Microsoft Excel by using Aspen Simulation Workbook (ASW). Lastly, the scenarios of the case study were run to determine the changes of the output variables by manipulating the input variables of the reactor.

3.2 Process Modelling

Process modelling is done by using process simulators. Although it was far from reality, the process simulators were designed to simulate processes and their behaviour, mainly for process control purposes. In other word, process simulators are used to mimic the real processes. Equipped with advance computation techniques, comprehensive thermodynamic packages and large component libraries, process simulators today provides reliable information of process design and operations. In this work, the case was modelled using Aspen Plus. The important steps to process modelling and simulation using process simulators include defining the chemical components, selecting the thermodynamic model and method, designing the process flow sheet by choosing proper operating units, determining plant capacity and setting up input parameters.

The steady state simulation model for methanol carbonylation process was carried out using Aspen Plus Simulation. The important steps to develop the simulation model was shown in Figure 3-1. In defining the process flow sheet, it is very important to define the unit operation and streams that's flowing to and from the unit operational in the process. Aspen Plus is a steady state chemical process simulator. It used unit operation blocks, which are models of specific process operation (reactors, heaters, pumps, distillation column, etc.). Then, these blocks were placed on a flow sheet, specifying material and energy streams. The model was selected from the Aspen Plus Model Library to describe each unit operation. Then, the labelled streams were placed on the process flow sheet and connected to the unit operation model to complete the steps. Then, the labelled streams were placed on the process flow sheet and connected to the unit operation model to complete the steps. Then, the chemical components in the process were specified. In this case, the chemical components that were specified are Methanol, Carbon Monoxide, Water, Hydrogen, Carbon Dioxide and Acetic Acid. All the chemical components were taken from the Aspen Plus databanks. Then, the thermodynamic model was specified to represent the physical properties of the components and mixtures in the process.

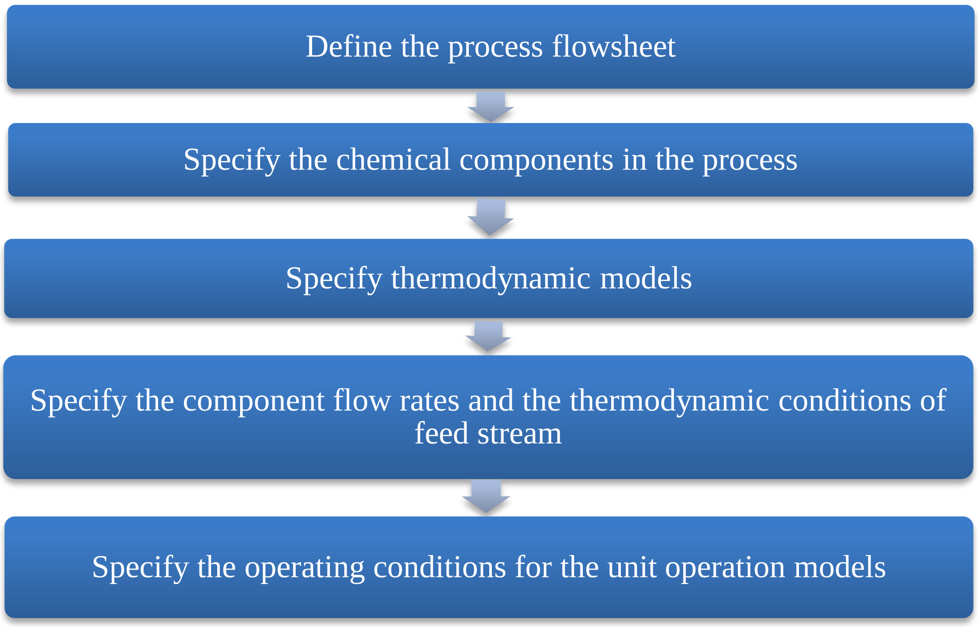

Figure 3-1: Steps in developing simulation models in Aspen Plus

3.3 Designing a Model of Methanol Carbonylation Process in Aspen Plus

The designed process flow diagram of acetic acid production via methanol carbonylation in Aspen Plus was shown in Figure 3-2 . It consists of the equipment and streams. The equipment selection is very important in order to meet the demand of the acetic acid production with high purity while minimized the cost of equipment used. This process was used the NRTL thermodynamic model and method because the components used were in the vapor and liquid phase (Job Lindenbergh, 1996).

In this case, the component compounds used in the simulation work are methanol, carbon monoxide, water, acetic acid, carbon dioxide and hydrogen. The raw materials used are methanol, carbon monoxide and water with mass fraction (w=1) respectively, whereas the output product from the process are acetic acid, carbon dioxide and hydrogen. The reaction section exists at a reactor (R-100), in which methanol was carbonylated with carbon monoxide and water to produce acetic acid with carbon dioxide and hydrogen gas as byproducts, and a distillation column (D-100) as purification of the product.

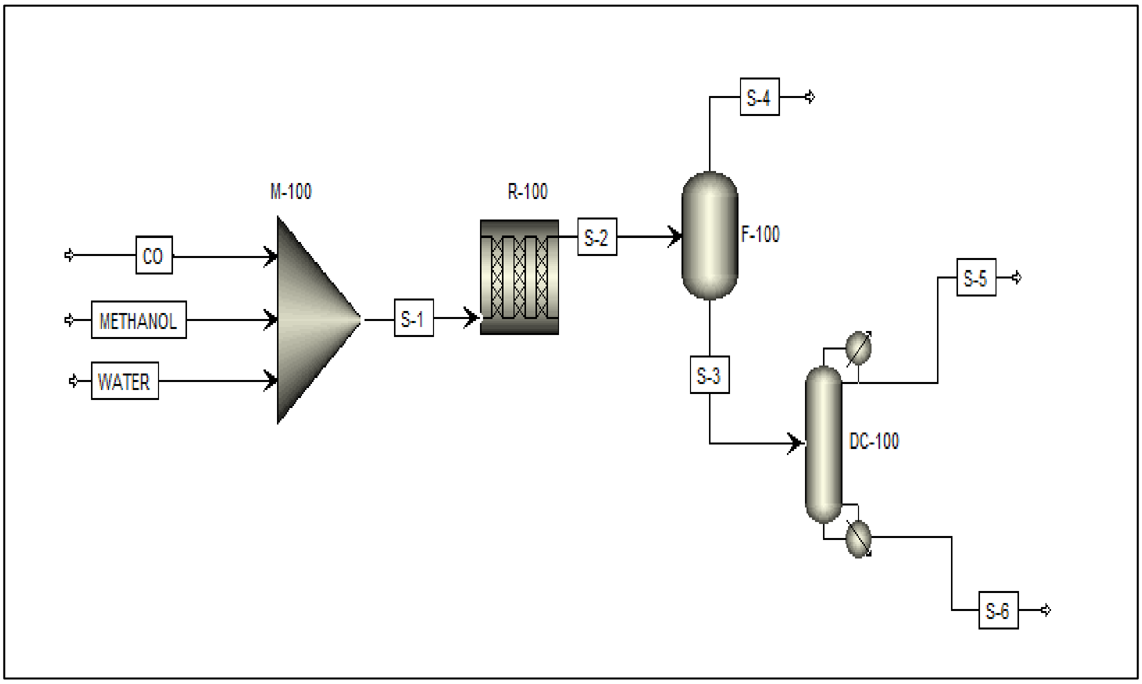

Figure 3-2: Simulation Model for Methanol Carbonylation Process

The equipments used in this model are mixer, plug flow reactor (R-Plug), flash distillation drum, and distillation columns (DSTWU). The operating conditions were set for methanol and carbon monoxide in gas phase 175 ^{o}C and 36 bar while for water in liquid phase is heating up at 80 ^{O}C and 36 bars (Job Lindenbergh et al.,, 1996). Every inlet feed mixtures must occur at a slightly higher pressure than our operating reactor condition to prevent backflow of feed mixtures to the mixer (Suzuki, I.Y, 1971). The properties of the materials involved in the process are given in Table 3-1.

Material	Formula	Molecular Weight (g/mol)	Melting Point (℃)	Boiling Point (℃)	Density (kg/l)(20℃)
Methanol	CH_3OH	32.04	-97.6	64.7	791.8
Carbon Monoxide	CO	28.0	-205	-191	0.001
Acetic Acid	CH_3COOH	60.1	17	118	1.049
Carbon Dioxide	CO_2	44.0	n.a	-79	0.001
Water	H_2O	18.0	0	100	1.000
Hydrogen	H_2	2.0	-259	-253	0.089

Table 3-1: Materials involved in the process (Job Lindenbergh, 1996)

3.4 The Reaction Kinetics of Methanol Carbonylation

The overall reaction in the reactor for the acetic acid synthesis via methanol carbonylation is represented simply by

$$2\,CO + H_2O + CH_3OH \rightarrow CH_3COOH + CO_2 + H_2$$

In aqueous media the rate is found to be dependent on carbon monoxide and methanol concentrations. However, with respect to a carbon monoxide concentration the rate is first order at low partial pressures of carbon monoxide and zero order at high partial pressure (above 3 bar) (Howard, 1993). In acetic acid media the rate shows a zero-order dependence with respect to methanol concentration, while the rate dependence with respected to carbon monoxide partial pressure is similar to that in aqueous media (Ind. Eng. Chem, 1989). The addition of hydrogen has no effect the reaction rate (Roth, J.F, Craddock, J.H., et al, 1971). The reaction rate for the production of acetic acid is given by equation (1) and (2), according to the describe kinetics.

$$R = k\,[CH_3I]\,[\text{Rh-complex}] \tag{1}$$

$$k = k_0\,exp\left(\frac{-E}{RT}\right), \tag{2}$$

Where, k_0 =3. 5 x 10^6 L/mol.sec and E = 61.5 KJ/mol. The reaction was found to be zero order with respect to both reactants (methanol & carbon monoxide). For this study, the pressure and temperature inlet stream of the reactor used is at 36 bar and 175°C. In the methanol carbonylation process, rhodium is used as a catalyst. But, for this case the catalyst is not considered in this process (Job Lindenbergh et al.,, 1996)

3.5 *Simulation of Reactor*

The simulation of the reactor begins by defining the components. The components used are methanol, carbon monoxide, water, acetic acid, carbon dioxide and hydrogen. The Figure 3-3 below showed the selection of the components used in Aspen Plus.

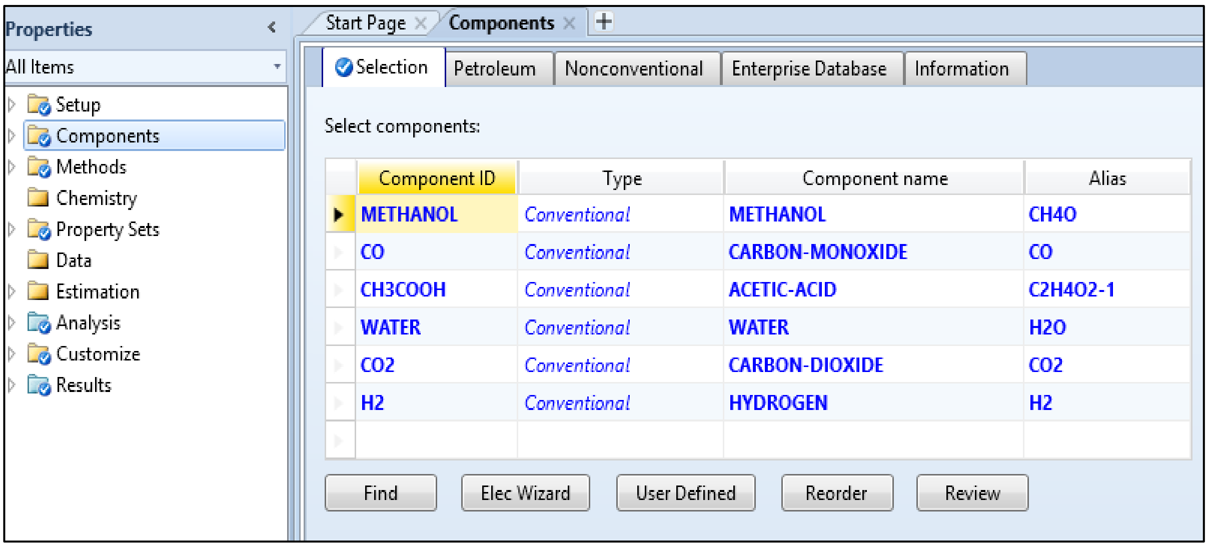

Figure 3-3: Selection of components in Aspen Plus

Next, the Rplug block model used in the Aspen Plus need specified reaction and kinetics. The Figure 3-4 and Figure 3-5 show the defined reaction and the specified kinetics data in Aspen Plus. In addition, the reactants and products of this reaction also were selected and the stoichiometric coefficient was specified. The specified stoichiometries coefficient was presented in Figure 3-6. There are several operating conditions of the reactor that need to specify such as the reactor type, number of tube, tube length and diameter and process stream. The specifications of the reactor that were used in the simulation were presented in Table 3-2.

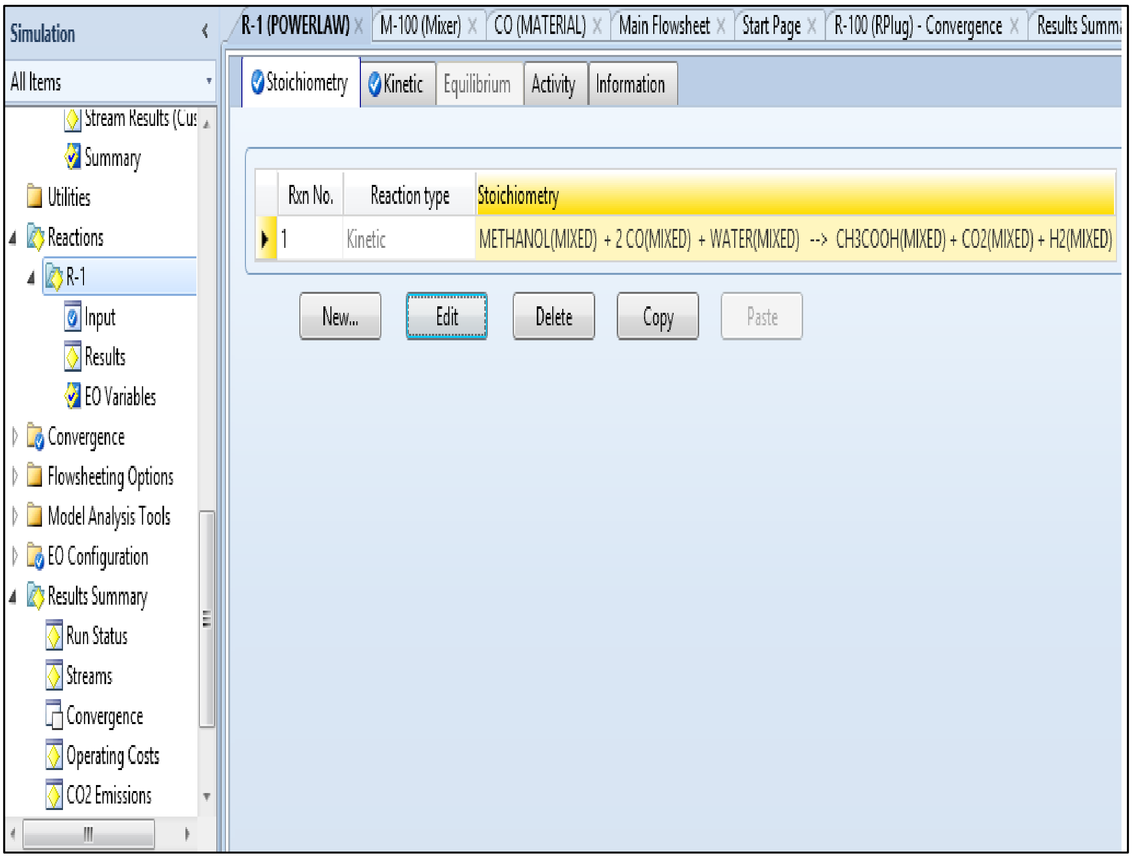

Figure 3-4: Reaction data of reactor in Aspen Plus

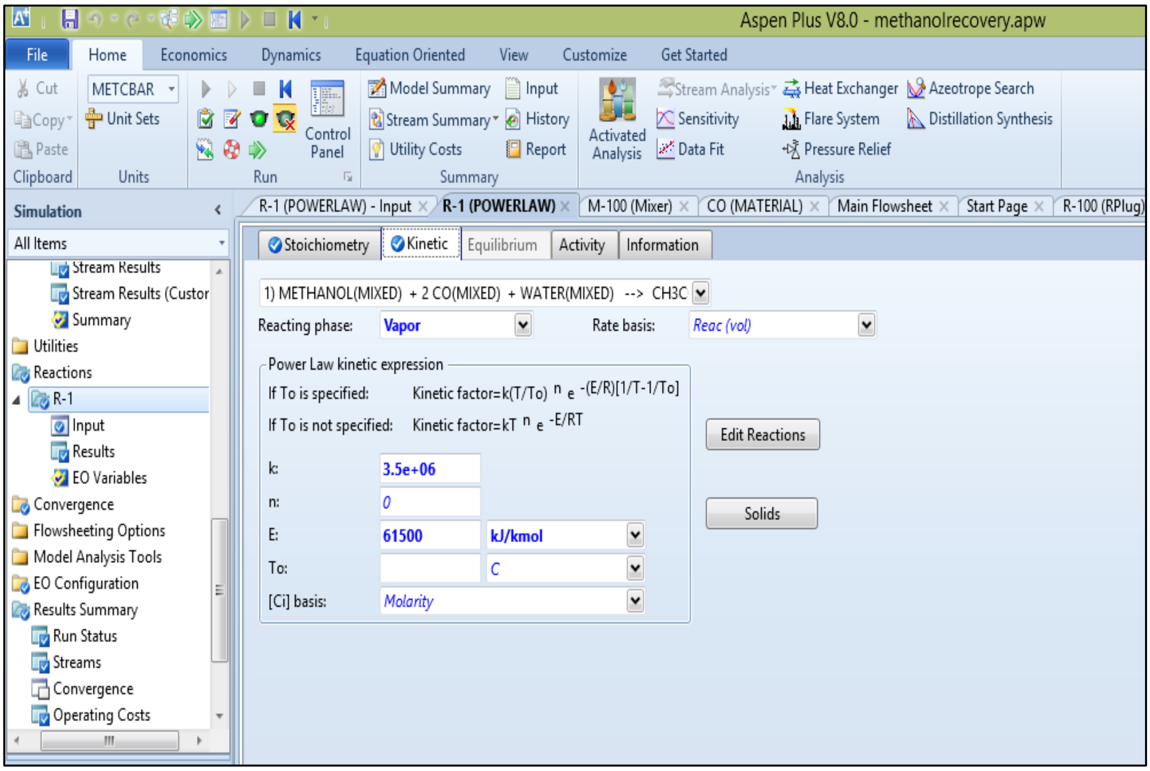

Figure 3-5: Specify kinetic data in Aspen Plus

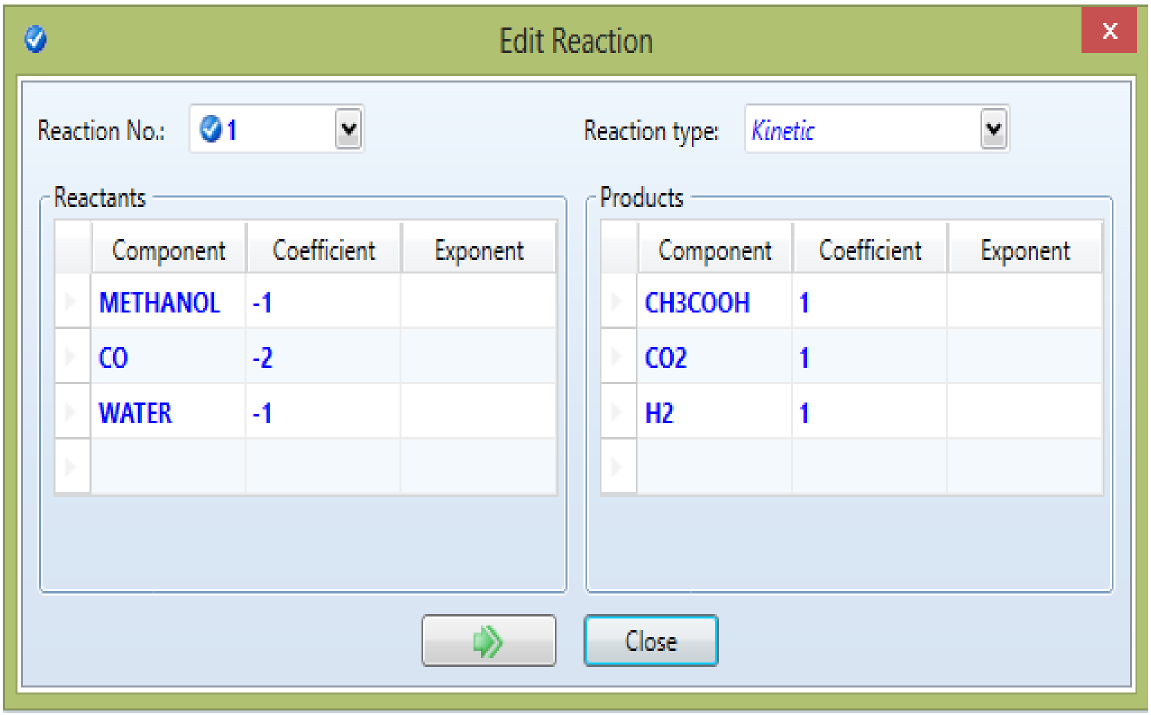

Figure 3-6: Specify stoichiometric coefficient in Aspen Plus

Specification	Reactor
Property method	NRTL
Reactor type	Reactor with specified temperature
No of Tube	300
Tube Dimension • **Length (m)** • **Diameter (mm)**	 2.3 22
Process Streams	Vapor-liquid

Table 3-2: Reactor Specification

3.6 Aspen Simulation Workbook (ASW)

Aspen Simulation Workbook is one of a methodology for developing the operating training simulators (OTS) of a chemical process. ASW provides seamless integration between AspenTech's engineering tools and Microsoft Excel, allowing us to deploy models to a wider range of users. Therefore, ASW is a powerful tool for creating convenient user interfaces to Aspen Plus models in Microsoft Excel. This makes it easy for other users without process simulation experiences to manipulate complex Aspen Plus simulation from Excel (Leviene & Tremblay, 2012). The Aspen Simulation Workbook interfaces can be created in just minutes by directly exporting data from the simulation (Aspen Simulation Workbook User Guide, V7.1, 2009).

3.7 *Connecting Model Simulation to Aspen Simulation Workbook*

After the development of the simulation model in Aspen plus was completed, the model was embedded in Microsoft Excel by using Aspen Simulation Workbook. The overall workflow to develop an interface in Aspen Simulation Workbook was shown in Figure 3-7.

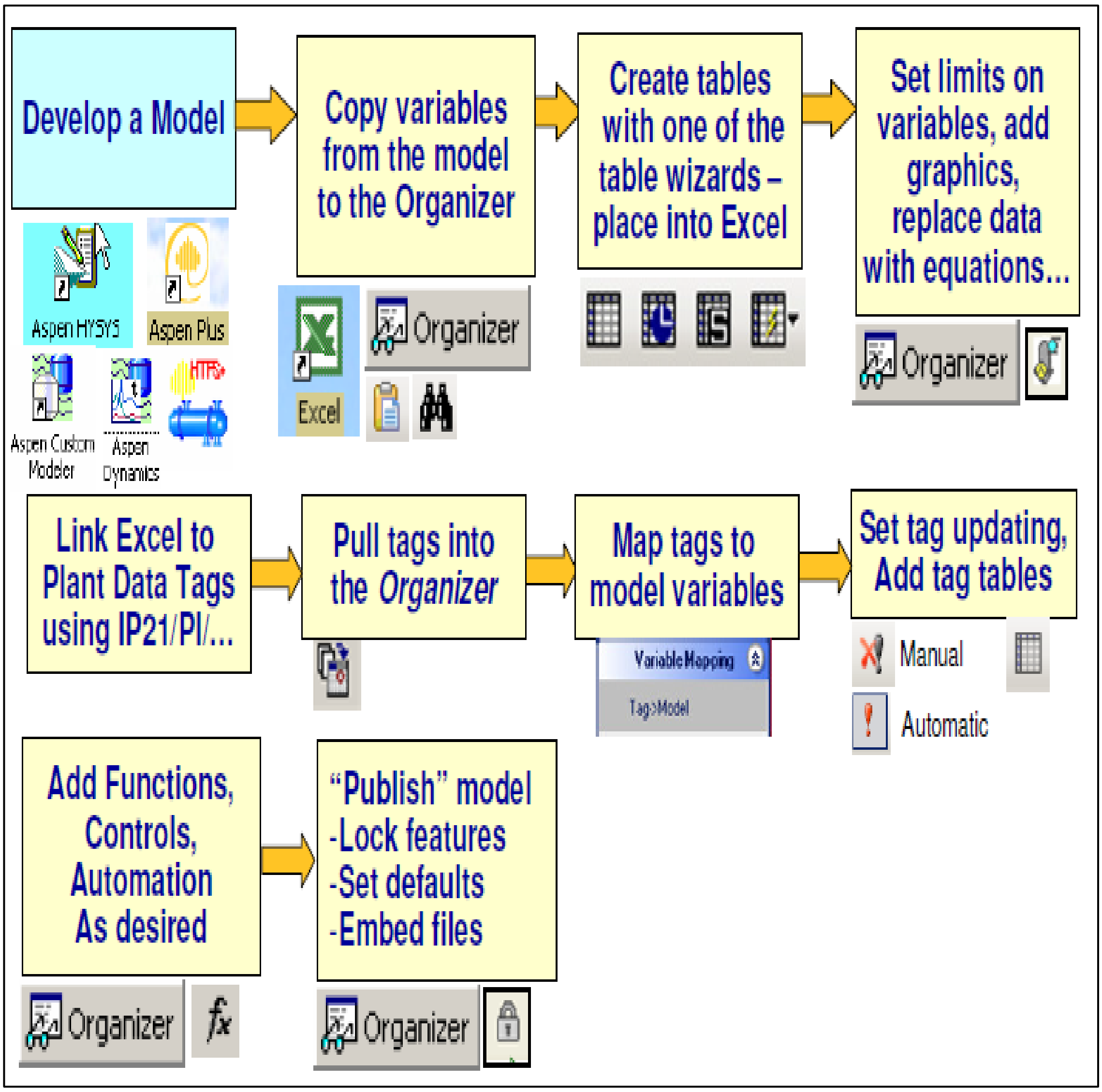

Figure 3-7: Aspen Simulation Workbook Workflow for Developing an Interface

In order to use and start Aspen Simulation Workbook, the first steps are familiarized with the Aspen Simulation Workbook Tab. The ASW tab is organized into five groups that show in Figure 3-8.

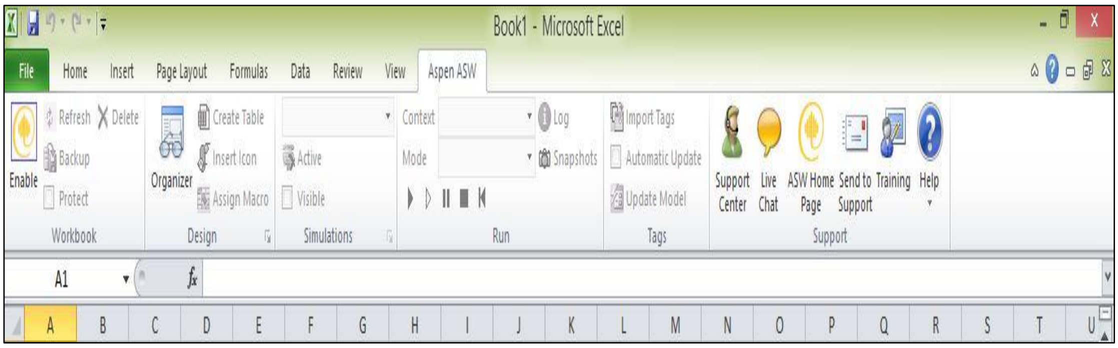

Figure 3-8: The ASW Tab opened in Microsoft Excel 2010

The following describes the general purpose of each tab:

- “Design”- To create and manipulate objects in the workbook
- “Simulation”- To determine which simulation is active if the workbook is connected to more than one
- “Run”- To run, pause, and reinitialize the simulation from Microsoft Excel
- “Tags”- To control tags that relate plant data to simulate variables
- “Support Group”- Several links to support, online training, and the AspenTech website.

Enable button was clicked to start the Aspen Simulation Workbook. After a few second, the button was changed to read Disable. The Organizer button from the tab was clicked and the symbol “+” at the top of the pane was selected to add a new simulation and a simulation from the computer was selected (Figure 3-9). The Figure 3-9 showed the circles mean that there are a few steps to link the simulation case study to ASW. The workbook has to link with the same simulation case study. For remote executive is to execute the workbook with the server.

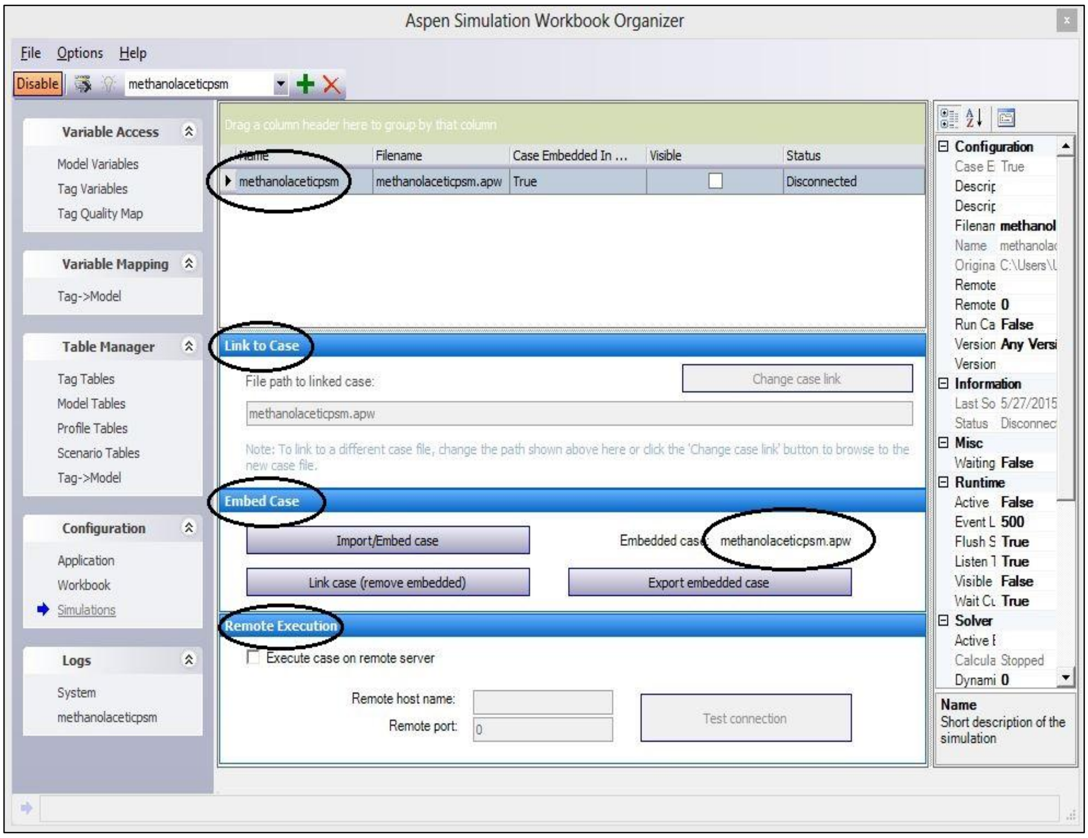

Figure 3-9: Adding new simulations in the Organizer pane.

Then, the variables from the model were copied to the Organizer in Excel. For most variables, using Copy/Paste is the best option for retrieving variables since it allows the Model Author to navigate to the variable using the native simulator user interface. Some variables, however, may not be exposed through the interface in a text-only format, making them inaccessible to the Copy/Paste mechanism. Users familiar with the variable explorer in Aspen Plus may prefer navigating through this browser instead of using Copy/Paste (Aspen Technology, 2004). Next, the simulation was opened and the variables were copied to link the model. For this case study of methanol carbonylation process, the variables of the reactor were selected. The variables were pasted in the Organizer pane, which is on “Model Variables” blank page that show in Figure 3-10.

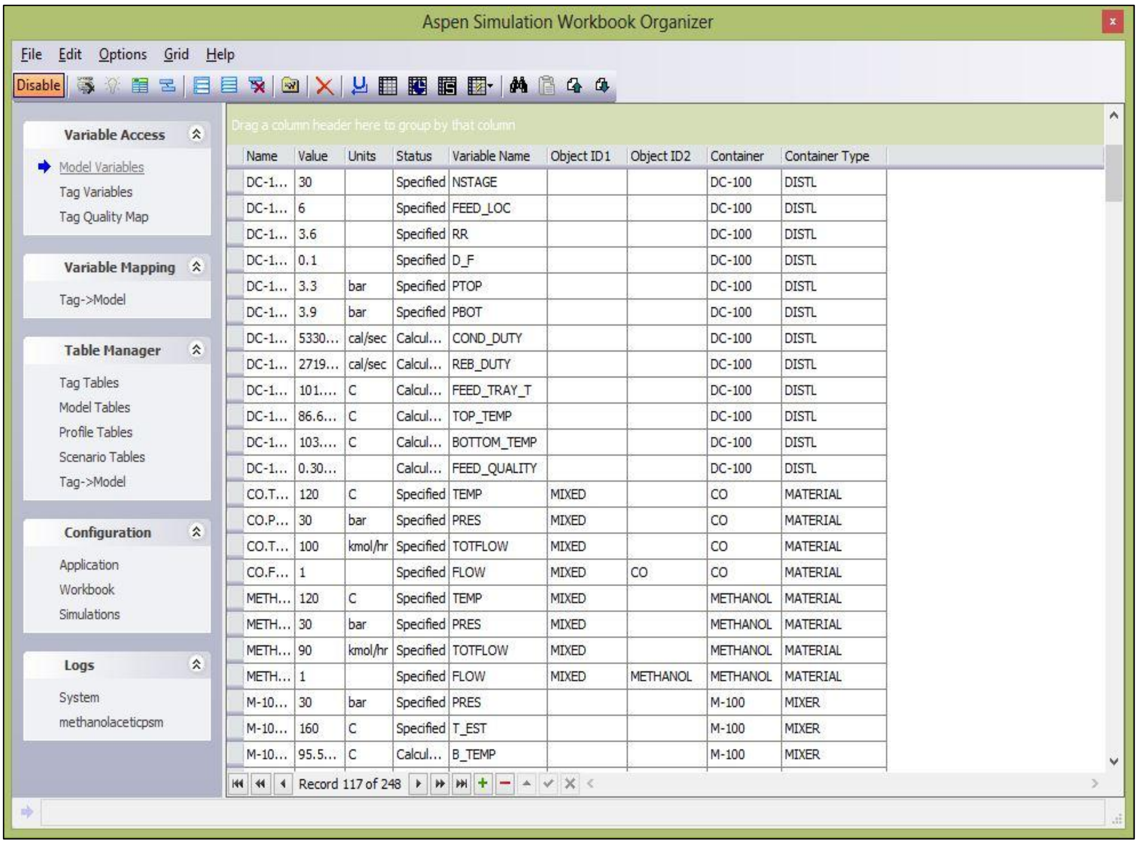

Figure 3-10: Adding the variables from the simulator to the worksheet

Next, the tables were created with one of the table wizards and then it was placed into Excel. Creating tables in ASW allow manipulating variables directly in Microsoft Excel without having to find them in the Aspen Plus model. Once the table was created, the cell values only need to be changed in workbook to adjust the model. The next step is to create tags. Tags allow users to input plant data into the simulations. It is possible to both map tags to the simulation and to do the reverse. Once the tags were created, it must be mapped to the simulation and ASW will automatically map any tags to model variables with the same name (Aspen Simulation Workbook User Guide, V7.1, 2009). Lastly, the simulation case file will be embedded in Excel. The files will save in the standard document management system, and the files will run remotely on a server.

3.8 Creating and Running Scenarios Table

Aspen Simulation Workbook includes a library of process equipment symbols. The process symbols are grouped into several categories based on the equipment function. (David Tremblay, 2014) To retrieve a process icon from the library the *Insert Icon* button was used. This tool opens the Insert Picture form. Browse to the desired icon and click the insert button to drop the icon onto the active Excel worksheet as shown in Figure 3-11.

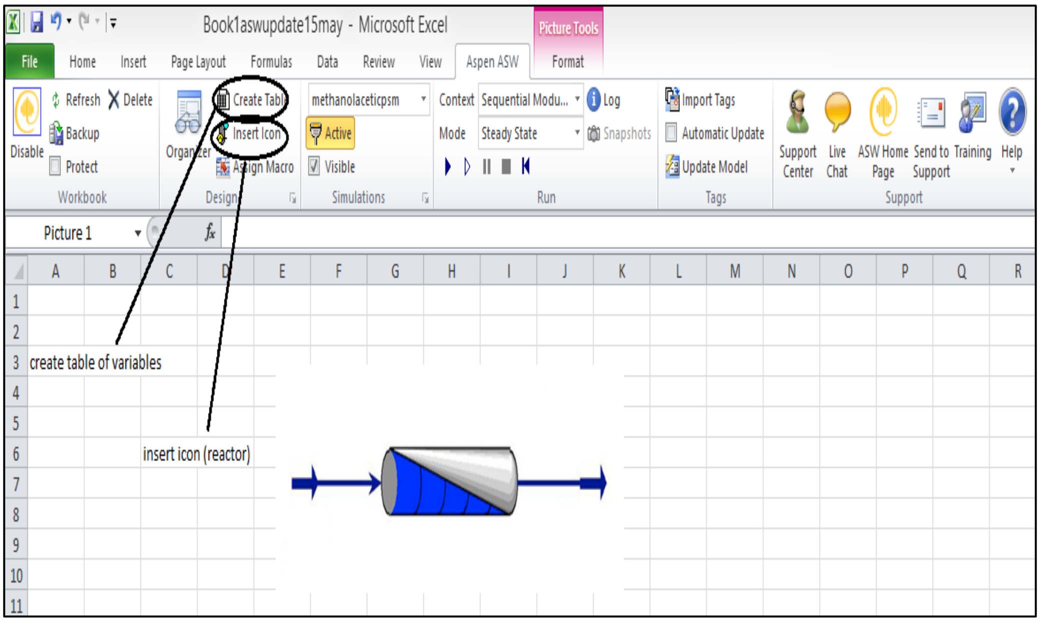

Figure 3-11: Adding a process icon in the library

After that, the variables were added in a worksheet. The table for the variables were created by click the *Create Table* button. The simulation workbook table wizard would appear. The table could design in any style and the column and row were set by adding the variables. The next step was creating scenarios table. The running scenarios could be defined in ASW using Scenario Tables. The scenario table was defined as a set of input variables and a set of output variables in a set of scenarios. Each row represents a scenario was defined by the values of the input variables. The ASW Organizer was opened and the Model Variables view in the left pane was clicked. At least one specified variable and at least one calculated variable was selected. The *Create Scenario Table* button was clicked and Create Scenario Table was selected as showed in Figure 3-12.

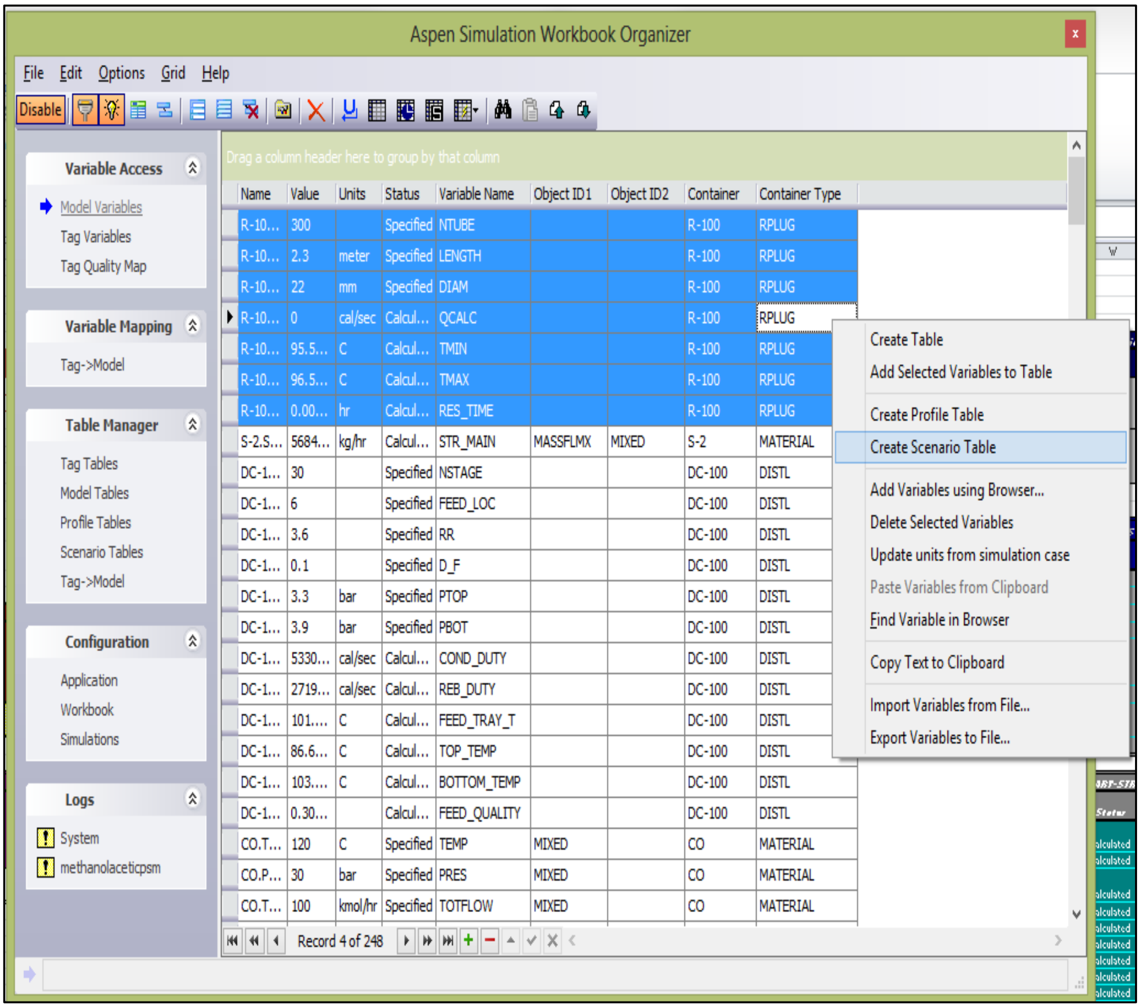

Figure 3-12: The scenario table button

When the create scenario table was selected, the cell was chosen to locate the scenario table. The Scenario Study Wizard window would appear. The table tab was used to specify the format for the table, and whether to include the title, column headings, and units. By default, the first row of the table would include the current values of specified and calculated variables. The Input Variables tab was used to specify the input variables. The Add button was clicked to add previously defined model variables by highlighting them and then Select button was clicked. The arrow buttons were used to order the variables. Next button was clicked. The Output Variables tab was used to specify output variables in the same manner. Then the Finish button was clicked to obtain the table.

3.9 Summary

This chapter presents the procedure to achieve the objective of this project. There are several steps to complete the task which are to develop a model, embedding simulation model in Microsoft Excel and running scenarios. Firstly, we need to develop a model in Aspen Plus Simulation in the complete process flow diagram of production of acetic acid via methanol carbonylation. The operating condition of each equipment was obtained from the journal. After running the simulation, we proceed with embedding the simulation model in Microsoft Excel by using Aspen Simulation Workbook. The simulation must be linked to Microsoft Excel. So, there are a few steps to insert the case simulation. After the simulation was connected to the Aspen Simulation Workbook, the variables that need to analyze in ASW was copied. The next step was running the scenario case which is we could show the equipment that we analyze in ASW and create a few tables that obtain the input and output variables of the reactor. We could develop the auto-run simulation by click on the image to run the simulation case study. In addition, we could use the steps to design the whole process from the simulation.

4 RESULT & DISCUSSION

4.1 Overview

This chapter was discussed on the result of this research, which is the development of an operator training simulator using Aspen Simulation Workbook on the reactor case study. The result of the process is obtained from the Aspen Plus Simulation and the result of running the scenario is obtained in the Microsoft Excel. For the result in running scenario parts, the input variables of the reactor are manipulated in order to get determine the changes of the output variables. In this study, the number of tube variable is manipulated in order to determine the changes of heat duty, residence time and also the production of acetic acid. The result obtained was discussed in this chapter.

4.2 The Simulation Model and Result Summary in Aspen Plus

The simulation model of the acetic acid production via methanol carbonylation was shown in Figure 4-1. From the Figure 4-1, the stream 1 is the inlet stream of the reactor whereas the stream 2 is the outlet stream of the reactor. The result of reactor stream obtained from the simulation was shown in Table 4-1. From the result, the total flow rate of the acetic acid production in the outlet stream of reactor is 29.46269 kmol/h. The overall result summary of all streams obtained from the Aspen Plus Simulation was shown in Table 4-2.

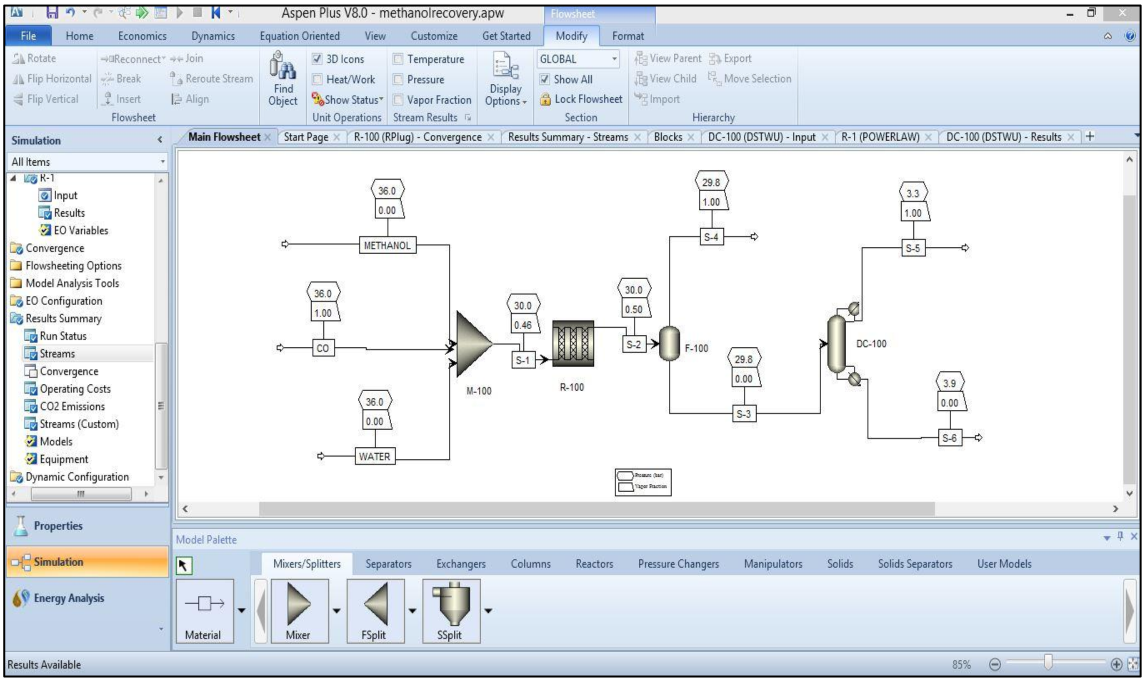

Figure 4-1: Simulation of Methanol Carbonylation Process

	Units	S-1	S-2
From		M-100	R-100
To		R-100	F-100
Substream: MIXED			
Phase:		Mixed	Mixed
Component Mole Flow			
METHANOL	KMOL/HR	100	70.53731
CO	KMOL/HR	90	31.07462
CH3COOH	KMOL/HR	0	29.46269
WATER	KMOL/HR	50	20.53731
CO2	KMOL/HR	0	29.46269
H2	KMOL/HR	0	29.46269
Mole Flow	KMOL/HR	240	210.5373
Mass Flow	KG/HR	6625.916	6625.916
Volume Flow	L/MIN	2145.241	2014.134
Temperature	C	126.8193	126.8193
Pressure	BAR	30	30
Vapor Fraction		0.4649351	0.4954965
Liquid Fraction		0.5350649	0.5045035
Solid Fraction		0	0
Molar Enthalpy	CAL/MOL	-45279.27	-55765.53
Mass Enthalpy	CAL/GM	-1640.079	-1771.94
Enthalpy Flow	CAL/SEC	-3018600	-3261300
Molar Entropy	CAL/MOL-K	-18.88487	-22.88017
Mass Entropy	CAL/GM-K	-0.6840367	-0.7270134
Molar Density	MOL/CC	0.00186459	0.00174217
Mass Density	GM/CC	0.0514776	0.0548285
Average Molecular Weight		27.60798	31.47146

Table 4-1: Result summary of reactor streams

Heat and Material Balance Table										
Stream ID		CO	METHANOL	S-1	S-2	S-3	S-4	S-5	S-6	WATER
From				M-100	R-100	F-100	F-100	DC-100	DC-100	
To		M-100	M-100	R-100	F-100	DC-100				M-100
Phase		VAPOR	LIQUID	MIXED	MIXED	LIQUID	VAPOR	VAPOR	LIQUID	LIQUID
Substream: MIXED										
Mole Flow	kmol/hr									
METHANOL		0.0	10 0.00 00	10 0.00 00	70 5 37 31	33 9 39 39	36 5 97 92	33 6 00 00	3 39 39 39	0.0
CO		90 0 00 00	0.0	90 0 00 00	31 0 74 62	2 43 30 06	30 8 31 32	2 43 30 06	6.2 20 8E-1 4	0.0
CH3COOH		0.0	0.0	0.0	29 4 62 69	25 3 14 26	4.14 84 32	0.0	25 3 14 26	0.0
WATER		0.0	0.0	50 0 00 00	20 5 37 31	13 3 05 67	7.23 16 45	1.3 30 57 E-7	13 3 05 66	50 0 00 00
CO2		0.0	0.0	0.0	29 4 62 69	8 52 03 86	28 6 10 65	8 52 03 86	1.3 41 7E-1 2	0.0
H2		0.0	0.0	0.0	29 4 62 69	0 33 40 41	29 4 29 29	0 33 40 41	9.0 77 7E-1 6	0.0
Total Flow	kmol/hr	90 0 00 00	10 0.00 00	24 0.00 00	21 0.53 73	73 6 88 06	13 6.84 93	34 7 28 74	38 9 59 32	50 0 00 00
Total Flow	kg/hr	25 20 9 36	32 04 2 16	66 25 9 16	66 25 9 16	28 91 7 63	37 34 1 53	11 20 9 97	17 70 7 66	90 0.76 40
Total Flow	l/min	15 52 5 28	93 4 30 53	21 45 2 41	20 14 1 34	65 7 58 25	27 59 4 82	53 96 4 27	34 8 28 52	15 9 84 90
Temperature	C	17 5.00 00	17 5.00 00	12 6.81 93	12 6.81 93	16 0.00 00	16 0.00 00	96 8 95 59	15 5.63 99	80 0 00 00
Pressure	bar	36 0 00 00	36 0 00 00	30 0 00 00	30 0 00 00	29 7 66 60	29 7 66 60	3.30 00 00	3.90 00 00	36 0 00 00
Vapor Frac		1.00 00 00	0.0	4 64 93 51	4 95 49 65	0.0	1.00 00 00	1.00 00 00	0.0	0.0
Liquid Frac		0.0	1.00 00 00	5 35 06 49	5 04 50 35	1.00 00 00	0.0	0.0	1.00 00 00	1.00 00 00
Solid Frac		0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Enthalpy	cal/mol	-2 53 50 .50	-5 22 16 .89	-4 52 79 .27	-5 57 65 .53	-7 41 06 .09	-4 33 79 .49	-4 81 30 .72	-9 21 70 .11	-6 72 75 .83
Enthalpy	cal/gm	-9 05 .03 88	-1 62 9.6 31	-1 64 0.0 79	-1 77 1.9 40	-1 88 8.3 75	-1 58 9.7 72	-1 49 1.1 01	-2 02 7.8 71	-3 73 4.3 76
Enthalpy	cal/sec	-6.33 76 E+5	-1.45 05 E+6	-3.01 86 E+6	-3.26 13 E+6	-1.51 69 E+6	-1.64 90 E+6	-4.64 31 E+5	-9.97 47 E+5	-9.34 39 E+5
Entropy	cal/mol-K	17 0 84 06	-4 5.8 52 07	-1 8.8 84 87	-2 2.8 80 17	-4 4.6 26 01	-5 .40 49 89	-2 9.4 03 92	-4 6.2 75 47	-3 5.9 30 77
Entropy	cal/gm-K	6 09 91 86	-1 .43 09 92	-.6 84 03 67	-.7 27 01 34	-1 .13 71 62	-.1 98 08 21	-.9 10 94 01	-1 .01 81 25	-1 .99 44 61
Density	mol/cc	9.6 61 66 E-4	0 17 83 85	1.8 64 59 E-3	1.7 42 17 E-3	0 18 67 65	8.2 65 40 E-4	1.0 72 58 E-4	0 18 64 34	0 52 13 25
Density	gm/cc	0 27 06 27	5 71 58 62	0 51 47 76	0 54 82 85	7 32 92 78	0 22 55 34	3.4 62 16 E-3	8 47 37 37	9 39 18 21
Average MW		28 0 10 40	32 0 42 16	27 6 07 98	31 4 71 46	39 2 43 31	27 2 86 62	32 2 78 65	45 4 51 67	18 0 15 28
Liq Vol 60F	l/min	80 3 36 70	67 2 24 33	16 2.60 27	16 2.23 22	52 1 40 21	11 0.09 19	23 5 94 93	28 5 45 29	15 0 41 67

Table 4-2: Result summary of streams

4.3 *Result in Aspen Simulation Workbook*

The developed operator training simulator using Aspen Simulation Workbook (ASW) in Microsoft Excel was shown in Figure 4-2. The operator training simulator was developed by developing the graphic user interface (GUI) in the Microsoft Excel. Once the interface was developed, the plant data have to activate to run the simulation with any changes of input variables by click *run simulation* button. The Aspen Plus simulation model of the methanol carbonylation case study can be open by click the *visible* button.

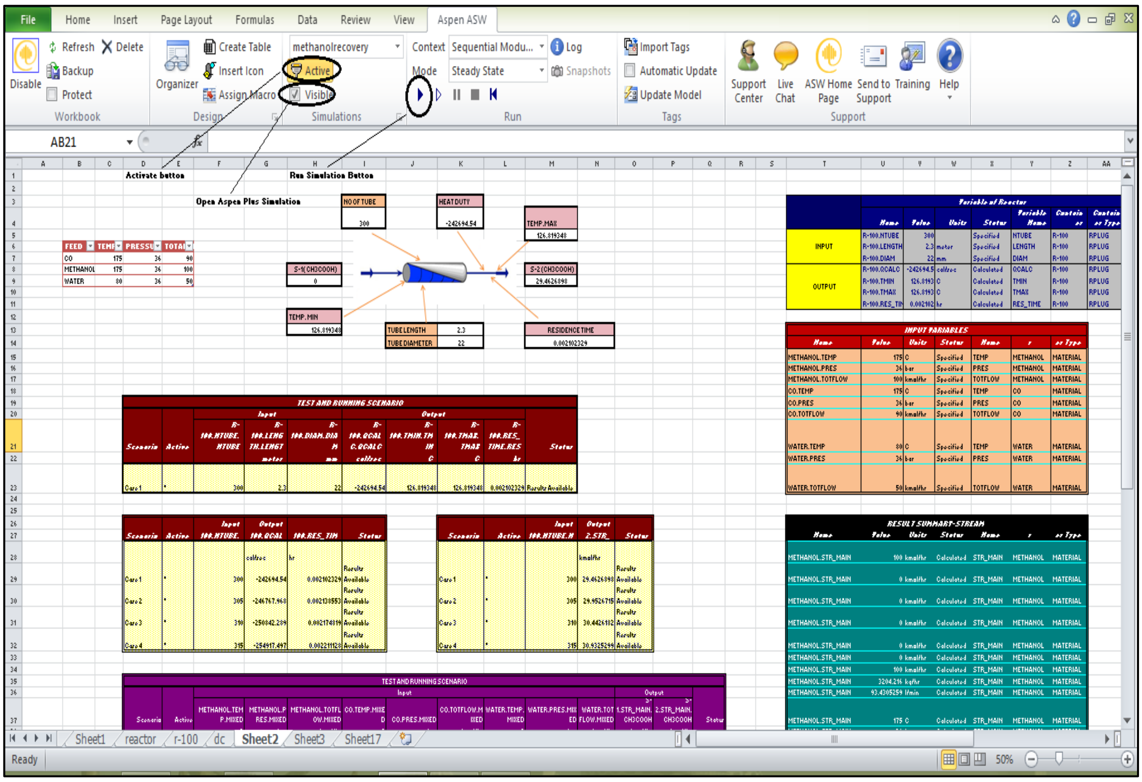

Figure 4-2: Graphical User Interface (GUI) of OTS in Microsoft Excel

The Figure 4-2 also showed the tables of data simulation process. By manipulating the value of input variables, the value of output also changed and have interfaced with the results from Aspen Plus simulations. It would make easier to handle the process plant with short time by Aspen Simulation Workbook compared to Aspen Plus simulation. (Aspen Technology, 2004).

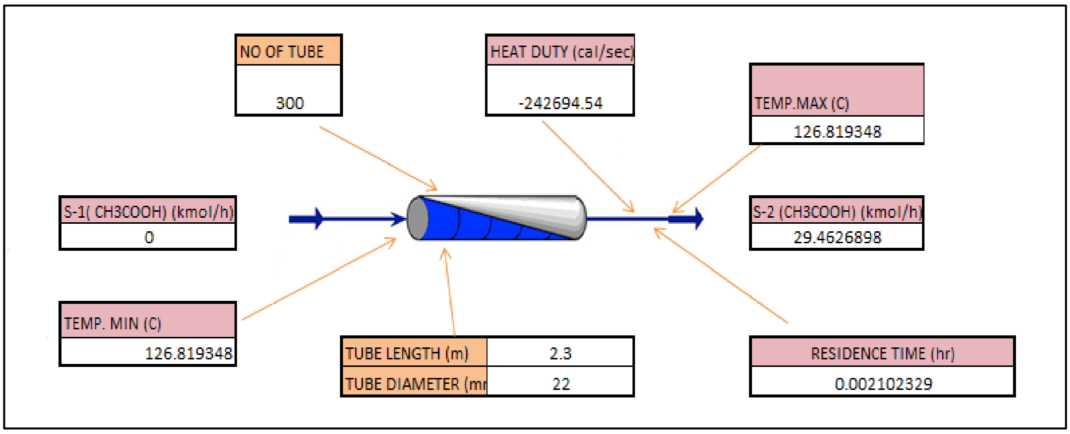

Figure 4-3: Graphical User Interface (GUI) of Reactor

The Figure 4-3 shown the graphic user interface of the reactor with the input and output variable. Based on the Figure 4-3, the orange boxes represent the input variables that could be manipulated for the reactor case study, whereas the pink boxes represent the output variables of the reactor. The input variables are the number of tubes, length of the tube, and diameter of the tube, whereas the output variables are heat duty, temperature minimum, temperature maximum, residence time and the acetic acid flow rate at stream 1 and stream 2. Since the reactor type used in the simulation is the reactor with specified temperature, the minimum temperature of the reactor will be same as the maximum temperature. All the variables is depends on the equipment that be used for Aspen Plus simulation.

This simulation workbook can be run by click on the image showed in Figure 4-3 and the output values will be changed by manipulating the input variables. The result obtained for input and output variables of the reactor was shown in Table 4-3 and Table 4-4 showed a scenario table for the value of input and output variables of the reactor. The reactant component variable to produce acetic acid was shown in Table 4-5 whereas the table showed the scenario table of input and output variables to obtain the acetic acid flow rate by stream 1 and stream 2.

	Variable of Reactor						
	Name	Value	Units	Status	Variable Name	Container	Container Type
INPUT	R-100.NTUBE	300		Specified	NTUBE	R-100	RPLUG
	R-100.LENGTH	2.3	meter	Specified	LENGTH	R-100	RPLUG
	R-100.DIAM	22	mm	Specified	DIAM	R-100	RPLUG
OUTPUT	R-100.QCALC	-242694.54	cal/sec	Calculated	QCALC	R-100	RPLUG
	R-100.TMIN	126.819348	C	Calculated	TMIN	R-100	RPLUG
	R-100.TMAX	126.819348	C	Calculated	TMAX	R-100	RPLUG
	R-100.RES_TIME	0.00210233	hr	Calculated	RES_TIME	R-100	RPLUG

Table 4-3: Variables of Reactor

TEST AND RUNNING SCENARIO									
		Input			Output				
Scenario	Active	R-100. NTUBE. NTUBE	R-100. LENGTH. LENGTH meter	R-100. DIAM. DIAM mm	R-100. QCALC. QCALC cal/sec	R-100. TMIN. TMIN C	R-100. TMAX. TMAX C	R-100. RES_TIME. RES_TIME hr	Status
Case 1	*	300	2.3	22	-242694.54	126.819348	126.819348	0.002102329	Results Available

Table 4-4: Run simulation section of Reactor

INPUT VARIABLES						
Name	***Value***	***Units***	***Status***	***Variable Name***	***Container***	***Container Type***
METHANOL.TEMP	175	C	Specified	TEMP	METHANOL	MATERIAL
METHANOL.PRES	36	bar	Specified	PRES	METHANOL	MATERIAL
METHANOL.TOTFLOW	100	kmol/hr	Specified	TOTFLOW	METHANOL	MATERIAL
CO.TEMP	175	C	Specified	TEMP	CO	MATERIAL
CO.PRES	36	bar	Specified	PRES	CO	MATERIAL
CO.TOTFLOW	90	kmol/hr	Specified	TOTFLOW	CO	MATERIAL
WATER.TEMP	80	C	Specified	TEMP	WATER	MATERIAL
WATER.PRES	36	bar	Specified	PRES	WATER	MATERIAL
WATER.TOTFLOW	50	kmol/hr	Specified	TOTFLOW	WATER	MATERIAL

Table 4-5: Reactant component variable

TEST AND RUNNING SCENARIO													
Scenario	Active	Input									Output		Status
		METHANOL. TEMP.MIXED C	METHANOL. PRES.MIXED bar	METHANOL. TOTFLOW.MIXED kmol/hr	CO.TEMP. MIXED C	CO.PRES. MIXED bar	CO. TOTFLOW. MIXED kmol/hr	WATER. TEMP.MIXED C	WATER. PRES.MIXED bar	WATER. TOTFLOW. MIXED kmol/hr	S-1. STR_MAIN. CH3COOH kmol/hr	S-2. STR_MAIN. CH3COOH kmol/hr	
Case 1	*	175	36	100	175	36	90	80	36	50	0	29.4626898	Results Available

Table 4-6: Run simulation section of reactant component

4.4 Test and Running Scenario

The reactor case study of this work is to determine the changes of heat duty of the reactor and the required residence time to achieve a 90 % conversion in the reactor by manipulating the variable of the number of tubes. The changes of the heat duty and residence time that affected by the number of tubes was shown in the Table 4-7 and the graph of the heat duty and residence time versus the number of tubes was shown in Figure 4-4 and Figure 4-5. Based on the Figure 4-5, it can be concluded that the higher number of tubes, the longer the residence time to achieve a 90 % conversion.

Scenario	Active	Input	Output		Status
		R-100.NTUBE. NTUBE	R-100.QCALC. QCALC Cal/Sec	R-100.RES_TIME. RES_TIME hr	
Case 1	*	300	-242694.54	0.002102329	Results Available
Case 2	*	305	-246767.968	0.002138553	Results Available
Case 3	*	310	-250842.289	0.002174819	Results Available
Case 4	*	315	-254917.497	0.002211128	Results Available

Table 4-7: Changes of heat duty & residence time

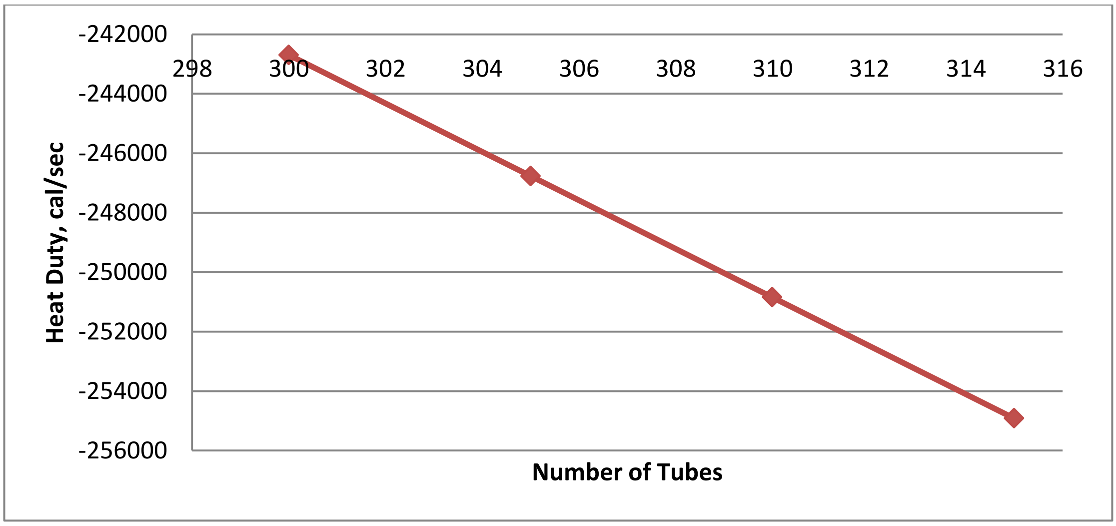

Figure 4-4: Trends of the heat duty

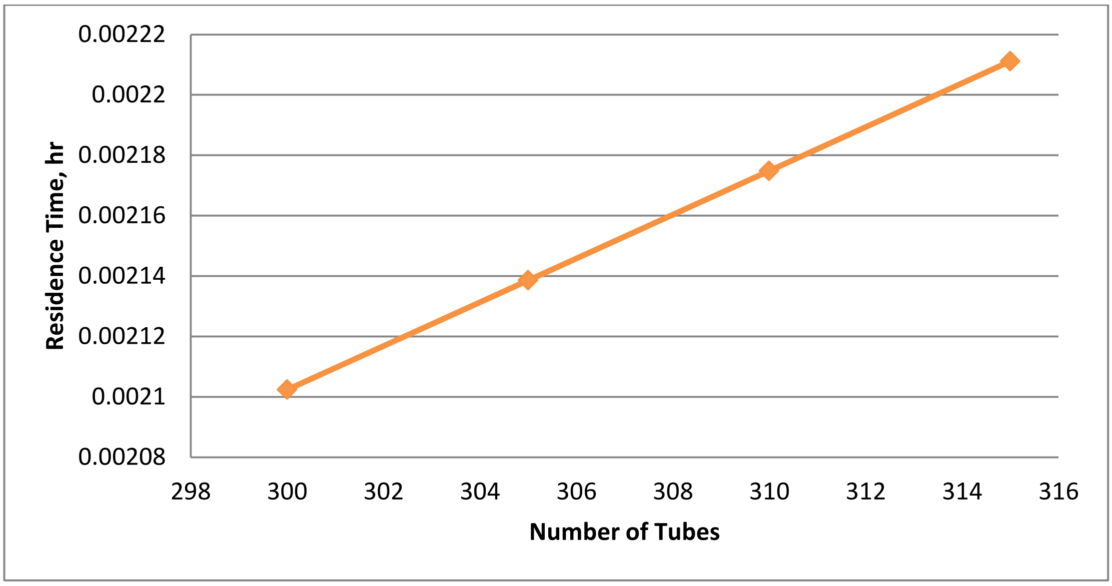

Figure 4-5: Trends of the Residence Time

Besides that, the other case study is to determine the changes of flow rate of acetic acid at stream 2 by manipulating the number of tubes in the reactor. The changes were shown in Table 4-8. The graph of the number of tubes versus the acetic acid flow rate was shown in Figure 4-6. From the Figure 4-6, the flow rate of the acetic acid will be increased when the amount of tube increase. Therefore, it can be concluded that the flow rate of acetic acid is proportional to the number of tubes.

Scenario	Active	Input	Output	Status
		R-100.NTUBE. NTUBE	S-2.STR_MAIN. CH3COOH Kmol/hr	
Case 1	*	300	29.4626898	Results Available
Case 2	*	305	29.9526715	Results Available
Case 3	*	310	30.4426182	Results Available
Case 4	*	315	30.9325299	Results Available

Table 4-8: Changes of heat duty & residence time

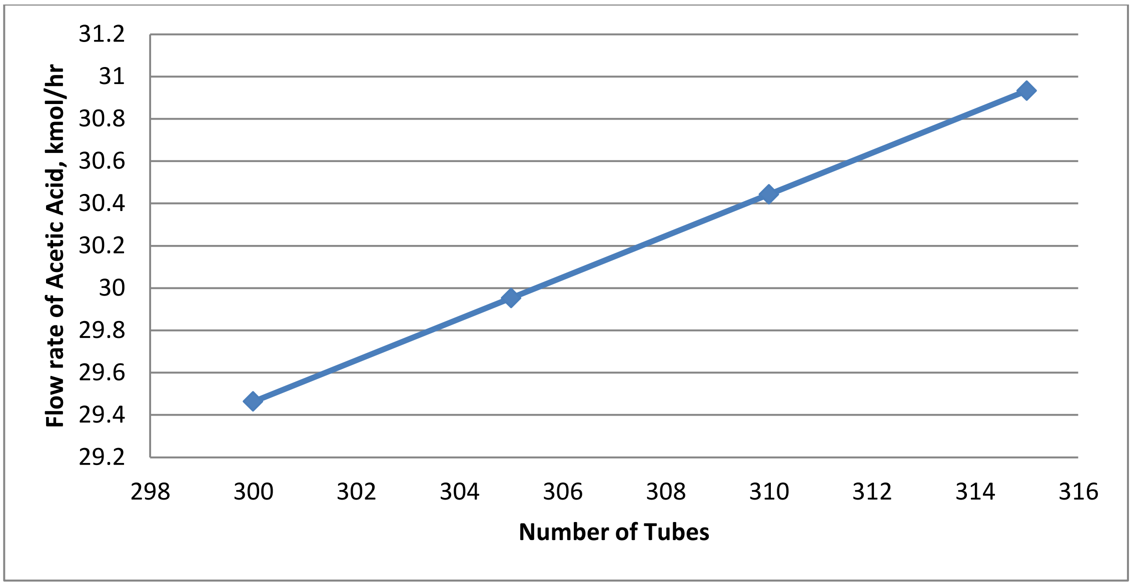

Figure 4-6: Trends of the Flow Rate of Acetic Acid.

5 CONCLUSION

5.1 Conclusion

As a conclusion, the objective of this research is achieved. An Operator Training Simulator (OTS) for acetic acid production via methanol carbonylation was presented in this work. The operating training simulator was developed with Aspen Simulation workbook software with extensive and versatile training capability, including simulation pause/run modes, simulation running mode control, user-friendly Graphic Uer Interface (GUI) instructor console, and extensive equipment of the library. These are the major features found in an OTS that are helpful in building an effective training program. The complete OTS tool therefore provides a simulated, though realistic, plant control room-like environment for the training of operators and engineers. This Aspen Simulation Workbook can be applied to the chemical industry, which is having the plant production by using this operator training. With integrated ASW software, process manufacturers can optimize their engineering, manufacturing, and supply chains. The advantages are they able to achieve operational excellence by increasing capacity, improving margins, reducing costs, becoming more energy efficient and also ensuring safety, In addition, this training also can be developed as an education purposes which is students will be trained to use the OTS in their study or design projects.

5.2 Recommendation

Some recommendations to upgrade the effectiveness of this research had been identified through the simulation of development operator training tools using Aspen Simulation Workbook of reactor case study, which by rigorous the model of simulation based on the method, types of equipment, and the properties of each component in dynamic models. Other than that, it is also recommended to analyze the sensitivity of the model towards Aspen Simulation Workbook in using the operator training simulator system.

REFERENCES

Aspen Technology, I. (2004). *Aspen Simulation Workbook User Guide.* 200 Wheeler Road, Burlington, Ma 01803,Usa: Aspen Technology, Inc., Burlington, Ma.

David Tremblay, V. M. (2014). A Brief Tutorial (Supplement To Training And Online Documentation). *Jump Start: Aspen Simulation Workbook In Aspen Plus® V8,* 3-10.

Fürcht, Á., Kovács, T., & Rabi, I. (2008). Implementation of operator training system in the MOL Danube refinery. MOL Scientific Magazin

Okapuu-von Veh, R., Marceau, R.J., Malowany, A., Desbiens, P., Daigle, A., Garant, E.,Gauthier, R., Shaikh, A., Rizzi, J.C.,(1996). Design and operation of a virtual reality operator-training system. IEEE Trans. Power Syst. 11, 1585–1591.

Jago, S. (2008). *Even Better Than The Real Thing.* United Kingdom: Institution Of Chemical Engineering.

Job Lindenbergh, E. S. (1996). *Preliminary Plant Design Chemical Process Technology.* Faculteit Der Scheikundige Technologie En Der Materiaalkunde.

Kbr, I. A. (2013). *Operator Training Simulators* . Retrieved March 31, 2014, From Http://Www.Kbr.Com/: Http://Www.Kbr.Com/Services/Advanced-Chemical-Engineering-Services/Operator-Training-Simulators/

Ltd, D. A. (2012). *Hyperion Has Delivered An Operator Training Simulator (Ots) At Lyondell Chemicals, France.* Retrieved March 30, 2014, From Www.Hyperionsystems.Net: Http://Www.Hyperionsystems.Net/En/News/News-Archive/124-Hyperion-Has-Delivered-An-Operator-Training-Simulator-Ots-At-Lyondell-Chemicals-France.Html

Management, Invensys Operations. (2010). Retrieved March 30, 2014, From Iom.Invensys.Com: Http://Iom.Invensys.Com/En/Pdflibrary/Whitepaper_Simsci_Benefitsofdynamicsimulationandoperatortrainingsystems_11-10.Pdf

Mhammed, J. O. (2005). Rapid Development Of Scenario-Based Simulations And Tutoring Systems. *Aiaa Modeling And Simulation Technologies Conference.* Collection Of Technical Papers.

Ming, R. W. (2003). Incident Prevention Training Simulator. *Computer Aided Chemical Engineering, Elsevier*.

Muravyev, A. &. (2007). Operator Training System For Hydrocracking Unit. *Aiche Annual Meeting,.*

Murugappan, R. (2009). *The Virtues Of Virtual : Tested And Approved.* The Star.

Preston, M. L. (1996). Cape-Crusading For Process Safety: An Industrial Perspective. *Computers & Chemical Engineering*, S1533-S1538.

Ross, M. (2013). Honeywell Process Solutions . *Improve Operator Training*, 1.

Lee, A.T., (2005). Flight Simulation – Virtual Environment in Aviation. Ashgate Publishing Ltd., London, UK

Kobayashi, T., Moridera, D., Komai, K., Fukui, S., Matsumoto, K., (1995). Fault diagnosisusing a diagnostic shell and its verification results by connecting to an operator training simulator. IEEE Trans. Power Syst. 10, 167–17Http://Www.Qvf.Com/Glass-Process-Systems/Recovery-Units/Qvf-Process-Acetic-Acid-Recovery.Html

Yang, S. H. (2001). Improve Safety Of Industrial Processes Using Dynamic Operator Training Simulators. *Process Safety And Environmental Protection*, 329-338.

Mani, S., Shoor, S.K., Pedersen, H.S., (1990). Experience with a simulator for trainingammonia plant operators. Plant/Operat. Prog. 9, 6–10

Dudley, T., Bouwer, W., de Villiers, P., Wang, Z., (2008). The thermal-hydraulic model for the pebble bed modular reactor (PBMR) plant operator training simulator system. Nucl. Eng. Design 238, 3102–3113.

Manca, D., Brambilla, S., Colombo, S., 2013. Bridging between virtual reality and accident simulation for training of process-industry operators. Adv. Eng. Softw.55, 1–9.

Balaton, M. G., Nagy, L., Szeifert, F. (2013), Operator training simulator process model implementation of a batch processing unit in a packaged simulation software. Computers and Chemical Engineering, 48, p. 335-344

Ferreira, S., Faezipour, M. (2012), Advancing the Development of System Engineers Using Process Simulators. Procedia Computer Science, 8, p. 81-86.

Bezzo, F., Bernardi, R., Cremonese, G., Finco, M., Barolo, M. (2004), Using process simulators for steady state and dynamic plant analysis. Chemical Engineering Research and Design, 82, p. 499-512.

Roe, A., Mason, J., Alamo, J. (2010), The role of simulator technology in operator training programs.

Kinetic Group, (2012), " Training Simulation" , http://www.kineticgroup.org.au/workforce-development-solutions/training-simulation/. Accessed on 28 March 2012.

GSE SYSTEM (2011/2012), Process Operator Training Simulator.1332 Londontown,Suite 200 Skyesvllle, Maryland, USA.

Invensys Operation Management (ION). (2010), The Benefits of Using Dynamics Simulation and Training Systems for Expanding Operator Knowledge and Understanding. Invensys Systems, SimSci.Esscor.

Aspen Technology, Inc. V7.2,. (2010). Aspen Plus,. Getting Started Building and Running a Process Model,.Burlington, MA.

Mohammed, J. L., Ong, J. C., Li, J. & Barbara Sorensen, H. (2005) Rapid development of scenario-based simulations and tutoring systems. Collection of Technical Papers - AIAA Modeling and Simulation Technologies Conference 2005.

Arc (2009) Honeywell I-MAC Capabilities Provide a Path to Operational Excellence. Dedham, USA, ARC Advisory Group.

Cameron, D., Clausen, C., Morton, W., Bertrand, B. & Rafiqul, G. (2002) Chapter 5.3: Dynamic simulators for operator training. Computer Aided Chemical Engineering. Elsevier.

Sebzalli, Y. M., Li, R. F., Chen, F. Z. & Wang, X. Z. (2000) Knowledge discovery from process operational data for assessment and monitoring of operator's performance. *Computers & Chemical Engineering,* 24**,** 409-414.

Seccombe, P. W. (2008) The Benefits of Using Dynamic Simulation and Training Systems for Expanding Operator Knowledge and Understanding.

Goh, S., Chang, B., Jeong, I., Kwon, H.-T. & Moon, I. (1998) Safety improvement by a multimedia operator education system. *Computers & Chemical Engineering,* 22**,** S531-S536.

Ahmad A.L., Low E.m., Abd. Shukor S.R (2010). Development of an Operator Training System for Gas Sweetening Plant.

Aspen Technology, Inc. V7.2,. (2010). Aspen Plus,. Getting Started Building and Running a Process Model,.Burlington, M

Chen Yuying., Yuan Guoqing., Chen Rongyao.,(1989). Kinetic Study of Carbonylation of Methanol to Acetic Acid and Acetic Anhydride Over A Novel Copolymer-Bound Cis-Dicarbonylrhodium Complex. Vol.7, No.3,226-231.

Ken-ichi Sano., Hiroshi Uchida., Syoichirou Wakabayashi..(1999). A New process for Acetic Acid Production by Direct Oxidation of Ethylene. 55-60.

Mohammadrezaei., Ali Reza.,Jafari Nasr., Mohammad Reza.,(2012). Kinetic Study, Modeling and Simulation of Homogenous Rhodium-Catalyzed Methanol Carbonylation to Acetic Acid. Vol.31,No.1, 57-73.

6 APPENDICES

APPENDIX A.1

A.1.1 Result summary-streams

RESULT SUMMARY-STREAM						
Name	**Value**	**Units**	**Status**	**Variable Name**	**Container**	**Container Type**
METHANOL.STR_MAIN	100	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	100	kmol/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	3204.216	kg/hr	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	93.4305259	l/min	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	175	C	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	36	bar	Calculated	STR_MAIN	METHANOL	MATERIAL
METHANOL.STR_MAIN	-1.43099201	cal/gm-K	Calculated	STR_MAIN	METHANOL	MATERIAL

RESULT SUMMARY-STREAM						
Name	**Value**	**Units**	**Status**	**Variable Name**	**Container**	**Container Type**
CO.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	90	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	90	kmol/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	2520.936	kg/hr	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	1552.52791	l/min	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	175	C	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	36	bar	Calculated	STR_MAIN	CO	MATERIAL
CO.STR_MAIN	0.609918559	cal/gm-K	Calculated	STR_MAIN	CO	MATERIAL
WATER.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	50	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	50	kmol/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	900.764	kg/hr	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	15.9849022	l/min	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	80	C	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	36	bar	Calculated	STR_MAIN	WATER	MATERIAL
WATER.STR_MAIN	-1.99446075	cal/gm-K	Calculated	STR_MAIN	WATER	MATERIAL

RESULT SUMMARY-STREAM						
Name	***Value***	***Units***	***Status***	***Variable Name***	***Container***	***Container Type***
S-1.STR_MAIN	100	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	90	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	50	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	240	kmol/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	6625.916	kg/hr	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	2145.24064	l/min	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	126.819348	C	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	30	bar	Calculated	STR_MAIN	S-1	MATERIAL
S-1.STR_MAIN	-0.684036735	cal/gm-K	Calculated	STR_MAIN	S-1	MATERIAL
S-2.STR_MAIN	78.2287608	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	46.4575216	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	21.7712392	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	28.2287608	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	21.7712392	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	21.7712392	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	218.228761	kmol/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	6625.916	kg/hr	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	2050.36609	l/min	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	126.819348	C	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	30	bar	Calculated	STR_MAIN	S-2	MATERIAL
S-2.STR_MAIN	-0.706283296	cal/gm-K	Calculated	STR_MAIN	S-2	MATERIAL

RESULT SUMMARY-STREAM						
Name	***Value***	***Units***	***Status***	***Variable Name***	***Container***	***Container Type***
S-3.STR_MAIN	37.7209953	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	0.396318228	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	18.9403372	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	18.6108136	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	0.684691271	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	0.026910631	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	76.3800663	kmol/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	2722.64533	kg/hr	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	63.7438732	l/min	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	160	C	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	31.0181267	bar	Calculated	STR_MAIN	S-3	MATERIAL
S-3.STR_MAIN	-1.20404688	cal/gm-K	Calculated	STR_MAIN	S-3	MATERIAL
S-4.STR_MAIN	40.5077655	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	46.0612033	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	2.83090198	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	9.61794718	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	21.086548	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	21.7443286	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	141.848695	kmol/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	3903.27067	kg/hr	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	2744.88468	l/min	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	160	C	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	31.0181267	bar	Calculated	STR_MAIN	S-4	MATERIAL
S-4.STR_MAIN	-0.138479876	cal/gm-K	Calculated	STR_MAIN	S-4	MATERIAL

RESULT SUMMARY-STREAM						
Name	***Value***	***Units***	***Status***	***Variable Name***	***Container***	***Container Type***
S-5.STR_MAIN	37.3437854	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	0.396318228	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	0	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	1.86108E-07	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	0.684691271	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	0.026910631	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	38.4517057	kmol/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	1237.86396	kg/hr	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	5976.80949	l/min	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	97.0119172	C	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	3.3	bar	Calculated	STR_MAIN	S-5	MATERIAL
S-5.STR_MAIN	-9.16E-01	cal/gm-K	Calculated	STR_MAIN	S-5	MATERIAL
S-6.STR_MAIN	0.377209953	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	8.84724E-14	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	18.9403372	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	18.6108134	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	9.41293E-13	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	6.38506E-16	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	37.9283606	kmol/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	1484.78137	kg/hr	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	29.4522459	l/min	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	151.450313	C	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	3.9	bar	Calculated	STR_MAIN	S-6	MATERIAL
S-6.STR_MAIN	-1.09413372	cal/gm-K	Calculated	STR_MAIN	S-6	MATERIAL

A.1.2 Equipment variables

INPUT VARIABLE-EQUIPMENT						
Name	***Value***	***Units***	***Status***	***Variable Name***	***Container***	***Container Type***
M-100.PRES	30	bar	Specified	PRES	M-100	MIXER
M-100.T_EST	175	C	Specified	T_EST	M-100	MIXER
R-100.NTUBE	300		Specified	NTUBE	R-100	RPLUG
R-100.LENGTH	2.3	meter	Specified	LENGTH	R-100	RPLUG
R-100.DIAM	22	mm	Specified	DIAM	R-100	RPLUG
F-100.TEMP	160	C	Specified	TEMP	F-100	FLASH2
F-100.VFRAC	0.65		Specified	VFRAC	F-100	FLASH2
DC-100.NSTAGE	46		Specified	NSTAGE	DC-100	DSTWU
DC-100.PTOP	3.3	bar	Specified	PTOP	DC-100	DSTWU
DC-100.PBOT	3.9	bar	Specified	PBOT	DC-100	DSTWU
DC-100.RECOVL	0.99		Specified	RECOVL	DC-100	DSTWU
DC-100.RECOVH	1E-08		Specified	RECOVH	DC-100	DSTWU

RESULT SUMMARY-EQUIPMENT						
Name	*Value*	*Units*	*Status*	*Variable Name*	*Container*	*Container Type*
M-100.B_TEMP	126.819348	C	Calculated	B_TEMP	M-100	MIXER
M-100.B_PRES	30	bar	Calculated	B_PRES	M-100	MIXER
M-100.B_VFRAC	0.464935121		Calculated	B_VFRAC	M-100	MIXER
M-100.LIQ_RATIO	1		Calculated	LIQ_RATIO	M-100	MIXER
R-100.QCALC	-178910.65	cal/sec	Calculated	QCALC	R-100	RPLUG
R-100.TMIN	126.819348	C	Calculated	TMIN	R-100	RPLUG
R-100.TMAX	126.819348	C	Calculated	TMAX	R-100	RPLUG
R-100.RES_TIME	0.002084552	hr	Calculated	RES_TIME	R-100	RPLUG
F-100.B_TEMP	160	C	Calculated	B_TEMP	F-100	FLASH2
F-100.B_PRES	31.0181267	bar	Calculated	B_PRES	F-100	FLASH2
F-100.B_VFRAC	0.65		Calculated	B_VFRAC	F-100	FLASH2
F-100.QCALC	104637.277	cal/sec	Calculated	QCALC	F-100	FLASH2
F-100.QNET	104637.277	cal/sec	Calculated	QNET	F-100	FLASH2