UNIVERSITI TEKNOLOGI MARA

CHE364

FINAL YEAR PROJECT (REPORT)

TITLE:

COCO SIMULATOR: A STEADY STATE FLOWSHEET SIMULATION ENVIRONMENT

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ABSTRACT

COCO simulator is an open-source chemical process simulation software which is accessible by anybody particularly students. It is claimed that this free software has similar capabilities like commercial software such as open flow sheet modelling environment incorporating unit operations, thermodynamic packages as well as reactions. In this project, the capabilities of COCO simulator are being investigated by simulating various chemical processes and then the results are compared head-to-head with those obtained by an established commercial process simulator. Several steps are used to explore this simulation, starting with the configuration and specification of the thermodynamic properties package (TEA), the reaction package (CORN), the unit operation collection (COUSCOUS) and the flow sheeting environment (COFE). The percentage error is calculated from the simulation results against those of Aspen Plus as the benchmark. The result shows the performance of COCO simulator is quite inconsistent. On one hand it gives a remarkable performance in dehydrogenation of toluene process with no errors but on the other hand it gives an erratic result in the separation of benzene and toluene process with a whopping 16.73% error. This anomaly must be investigated further in the future and it does not necessarily mean that COCO simulator is an incompetent software since this is just a preliminary study. Therefore, it is concluded that free and open-source software such as the COCO simulator is indeed able to perform similar tasks like commercial software such as Aspen Plus and thus it has some potential as alternative simulation software in chemical engineering education although its accuracy in certain task is left much to be desired.

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1. BACKGROUND OF STUDY

1.1 Introduction

Process simulation is defined as a practice to stimulate a process using a model system before the actual process being work. Almost all companies especially in processing plant in the industry will do the process simulation in order to determine the error of each process, the amount of the production will be collected, how the process work etc. Thus, the company can prevent earlier the causes that might be occurred before the actual process done.

Many types of software that being used in worldwide for the process simulation. Basically, there are two types of software that can be categorized, which are commercial software and open-source software. Commercial software is known as a software that has source code for specific group only, such as team or organization. Example of commercial software is Aspen Plus. Meanwhile, open-source software can be defined as a code software that is being made to be use by everyone without any charges. This software can be used to modify, enhance, and also distribute, same goes like commercial software. One of the examples for open-source software is COCO Simulator.

COCO Simulator is a group of software that can be used in chemical engineering for setting up a steady state flowsheet simulation for chemical processes. This software is a sequential simulation process modelling environment. COCO Simulator was originally developed as a test for CAPE-OPEN modelling software. CAPE-OPEN (Computer Aided Process Engineering) is defined as a programming interfaces for aided process engineering. It is used mainly in the process engineering, which is it can be enables structured communication with the products created by ourselves. COCO Simulator consist of four (4) components in order to allow the user to setting up the flowsheet and the calculation. The first one is Flowsheeting Environment (COFE). COFE is an intuitive chemical flowsheet graphical user interface. This component has an automatic stream sequence solution algorithm. The flowsheet from COFE consist of stream properties, manages unit conversion, and offers plotting facilities. The second component is Thermodynamic for Engineering Applications (TEA). TEA can be referred on thermodynamic library from ChemSep and it also consists of over 430 chemical reactions in a data bank. The next component is CAPE-OPEN Unit Operation Simple Package (COUSCOUS). This component has several common types of equipment, such like the splitter, mixer, heat exchanger, pumps, and reactors. The last component is CAPE-OPEN Reaction Packages (CORN). This facility will specify the types of kinetic or equilibrium reaction to be occurred during the process simulation.

1.2 Problem statement

Commercial software that is usually used for simulation processes in universities or institutions requires expensive license that needs be renewed every year. This could put a stress on their already tight budget constraints. In addition, many students may not be able to use it as frequently as they wish due to time limitations, since students are restricted to use only during normal laboratory hours. So, this situation could have an impact on the effectiveness of their work. It could be worse if the assignment requires solely the use of software to be completed.

1.3 Objective

The aim of this project is to investigate the effectiveness of COCO simulator in simulating steady state chemical processes and to evaluate its potential as an alternative process simulation software.

2. METHODOLOGY

In this project, the simulations were performed using the COCO Simulator software. COCO (CAPE-OPEN to CAPE-OPEN) is a free chemical process simulation environment that use the CAPE-OPEN protocol (Computer Aided Process Engineering in Open Interfaces). This protocol allows the sharing of a shared interface between unit operations and thermodynamic models, consistent with most simulation environments available on the market. Several steps can be taken to make this simulation work in order to obtain results for the project.

2.1 TEA Property Packages

Thermodynamics framework must be specified first using TEA (Thermodynamics for Engineering Applications) before the simulation is started. For this, a ConfigureTEA utility from COCO start menu is used and this will open the TEA configuration window directly as shown in Figure 2.1.1.

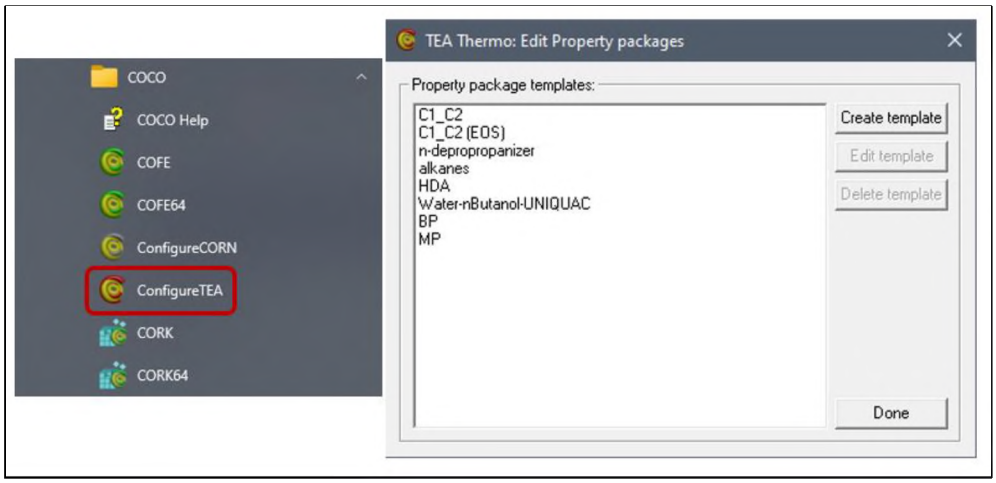

Figure 2.1.1: ConfigureTEA from COCO Start Menu

In this window, a property package can be created by clicking on the Create template button. The TEA package configuration dialog will appear as shown in Figure 2.1.2. First, it is necessary to determine the name and description of the property package. The compounds selected for the property package can then be added by clicking the Add button.