INTEGRATED TOOL FOR ASSESSING SUSTAINABILITY INDEX OF DISTILLATION COLUMN SYSTEMS

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Abstract

This paper presents the application of the integrated tool for assessing the sustainability index of distillation column systems. Sustainability tool was developed to assess and improve the sustainability of a process. However, the current developed sustainability tools are only based on the one-dimension analysis. In this study, a new integrated tool for assessing sustainability index of distillation column systems is developed. The advantage of this tool is that the calculation of the sustainability index will consider three different indices simultaneously, which are one-dimension, two-dimension and three-dimension indices. By using the developed tool, the comparison between those three types of sustainability indices can be done in an easy and systematic manner. The framework of the developed integrated sustainability tool consists of four parts: introduction, components selection, data input and analysis. The objective of the first part is to introduce the user to the distillation column process. Then, the users have to select components which are involved in the process in the second part. Next, in the third part the users need to key in the necessary data, such as feed and product flow rates and composition, energy for condenser and reboiler, and others required data. The fourth part is the analysis part, which the objective is to analyse and display the calculated value of the sustainability indices. The application of this tool is illustrated using the separation of benzene and toluene with a single distillation column. The data required for the tool was obtained from the highest point of the driving force that used to design the distillation column. It is shown that the tool able to analyse three different sustainability indices simultaneously in easy and systematic manner.

Keywords: Sustainability, index, integrated tool, distillation column systems.
1. Introduction

Sustainability has turning out to be a major issue nowadays. This issue has been discussed widely in public and become a global concept that is used to discuss in various fields including chemical processes. According to the report of the 1987 World Commission on Environment and Development, sustainability can be defined as “development that meets the needs of the present without compromising the ability of future generations to meet their own needs” [1]. A full concept of sustainability has to aim at sustaining human freedoms, instead of at our ability to fulfil our felt needs.

Sustainability is based on balancing three principal objectives; environmental protection, economic growth, and societal equity. Metrics and indicators are used to assess the sustainability performance of a process or a system, in order to evaluate the progress toward enhancing the sustainability, and also to assist decision makers in evaluating the alternatives. According to the Venn diagram in Fig. 1, one-dimensional (1D) index indicates the sustainability criteria individually for the process or design. While two-dimensional (2D) index provides information simultaneously about two dimensions of sustainability: socio-environmental (equitable), socio-economic (bearable), or environmental-economic (viable). Though, the three-dimensional (3D) index, one that covers all three criteria is known as sustainable. There were many computers aided or tools have been developed to simplify and make the sustainability analysis become easier. Shadiya and High for example, developed Sustainability Evaluator, a tool for evaluating processes for sustainability [2]. However, the developed tool is only based on the single analysis which is the 1D sustainability analyses.

![Fig. 1. Venn diagram for sustainability criteria.](image)

The objective of this paper is to present the application of a new integrated tool for assessing the sustainability indices of distillation column systems. The novelty of this tool is that it integrates three different sustainability analyses (1D, 2 D and 3D) into one single analysis. This integrated tool is able to analyse the sustainability for chemical processes such as distillation column system. In this paper, the capability of the developed tool is tested in analysing the sustainability of the separation of benzene and toluene in a distillation column system.
2. Integrated Tool Overview

The framework of the developed tool for sustainability analysis of distillation column systems was implemented into an excel-based software which integrates three types of sustainability indices (1D, 2D and 3D) into a single analysis.

Figure 2 shows the start menu that has been created as the user interface (UI) for this calculator. From the starting point, the user can choose two different systems: i) a single reactor system and ii) a single distillation system by clicking on the corresponding button. However, this paper only presents the application of distillation column system. Other than that, on the left side of UI, there are three info buttons which are “Software Overview”, “User’s Manual” and “Tutorial” to help user to understand about this integrated tool. The developed sustainability tool can be obtained from the corresponding author.

![Start menu user interface of the integrated tool.](image)

2.1. Integrated tool implementation

The analysis starts by click the button either the ‘A Single Reactor System’ button or ‘A Single Distillation Column System’ button. For this paper, the user should click an ‘A Single Distillation Column System’ button. Then, the main menu for a single distillation column sustainability analysis will appear which consists of four different parts: Introduction, Problem Definition, Data Input and Analysis as shown in Fig. 3. In order to calculate the sustainability for this distillation column system, the user needs to key in all information needed about the distillation column system in sequential manner.

2.1.1. Part 1: Introduction

Figure 3 shows the main menu for the distillation column system at which the user will directly see the Introduction part. In this part, some process description about the distillation column analysis is briefly explained. Other than that, the process flow diagram of the distillation column system is also shown to help the user to understand the system.

2.1.2. Part 2: Component selection

The next part of the integrated tool is the “Component Selection” part as shown in Fig. 4. The purpose of this part is for the user to select all the components involved in the distillation column system. Basically, there are three main...
component streams for a distillation column system; feed, distillate and bottom streams. The user is compulsory to select component for all those streams from the provided components list before proceeding to the next part.

2.1.3. Part 3: Data input

The third part of this tool is called the Data Input. In this part, the user is required to key in all the data needed to analyse the sustainability of the distillation column system. All the data needed in this part are entered manually, one by one in the data input interface as shown in Fig. 5. Flow rate and composition for each stream, energy and others data are needed in this part to analyse and calculate the sustainability index for the distillation column system. These data can be obtained from the process simulator such as Aspen HYSYS or Aspen Plus.

Fig. 3. Part 1 in the main menu of the integrated tool.

Fig. 4. Component selection interface of integrated tool.
2.1.4. Part 4: Analysis

When the calculation process is done, the analysis interface will appear as shown in Fig. 6. The analysis is able to evaluate and validate the effect of the process to the environment. When the value approaches zero, it shows that the distillation column system is more sustainable.

Three dimensions (1D, 2D and 3D) of sustainability indices are analysed simultaneously. For each sustainability index, the analysis is performed with the corresponding indicators. For 1D index analysis, the indicators provide information for one dimension of sustainability only, either on the economic, environmental or
societal. There are five indicators used to determine the 1D index which are economic indicator (economy), environmental and resource usage indicator (environmental) and, inherent safety and health risk indicator (society) [2]. For 2D index, the indicators are based on two simultaneous sustainability dimensions of economic-environmental, socio-economic and socio-environmental. However, only economic-environmental indicators are used for the 2D sustainability indexes which are mass intensity, water intensity and energy intensity [3]. For 3D index, all indicators must consist of all three dimensions of sustainability. Four indicators are used to determine the 3D indexes which are material intensity, energy intensity, potential chemical risk and potential environmental impact [4].

3. Integrated Tool Application

The application of the integrated tool is illustrated using the separation of benzene and toluene mixture in a single distillation column system. The data required for this analysis are taken from the highest point of the driving force that used to design the distillation column [5].

In the first part, the introduction of the separation process by using distillation column is described. Then, in part 2, the components selection for the feed, distillate and bottom stream is executed. For this case study, benzene and toluene are selected for the feed stream. Since there is no such a perfect separation, both components were chosen as distillate and bottom products. Next in the part 3, the mass flow rates and component mass fraction in each stream are specified. After that, the condenser and reboiler heat duty are specified. Some other data are also needed such as temperature, pressure, material used, type of equipment used, the process reliability, duration used of the component per day and the medium used for releasing the waste. The data for the separation of the benzene and toluene were obtained from the highest point of driving force that used to design the distillation column. All the data are listed in the Table 1. After all data have been specified, the “calculate” button can now be clicked to allow the tool to calculate the 1D, 2D and 3D sustainability indices. Lastly, the analysis part will appear to display the results of the calculated indices as shown in Figs. 7, 8 and 9. It can be seen that this tool successfully able to calculate three different dimensions of sustainability indices simultaneously in an easy and systematic way.

| Table 1. Data used for sustainability analysis of separation of benzene and toluene mixture. |
|----------------------------------|-------------------|-------------------|-------------------|
| Stream                          | Flow rate       | Feed             | Distillate        | Bottom            |
|                                 | 10000 kg/hour   | 8061 kg/hour     | 1939 kg/hour      |
| Mass Composition                | Benzene         | 0.8              | 0.99              | 0.01              |
|                                 | Toluene          | 0.2              | 0.01              | 0.99              |
| Energy                          | Condenser        | 782640 kJ/hour   |
|                                 | Reboiler         | 881940 kJ/hour   |
| Other Data                      | Product Stream   | Distillate       |
|                                 | Duration of Usage| 8 hours          |
|                                 | Receiving Medium | Water            |
|                                 | Type of Equipment| Heat exchangers, pumps, towers and drums |
|                                 | Material for Construction| Carbon Steel |

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Fig. 7. 1D analysis of separation of benzene and toluene mixture by using integrated tool.

Fig. 8. 2D analysis of separation of benzene and toluene mixture by using integrated tool.

Fig. 9. 3D analysis of separation of benzene and toluene mixture by using integrated tool.
4. Conclusions

An integrated tool was successfully developed that able to calculate sustainability index. The advantage of this tool is that it able to analyse three different dimensions (1D, 2D and 3D) of sustainability indices simultaneously. This tool is able to analyse distillation column system through the application of the separation of benzene and toluene mixture with a single distillation column system. By decomposing the tool into four main frameworks allowed the integrated tool to analyse the sustainability of the distillation column system in an easy, systematic and efficient manner. This excel-based sustainability tool is a user friendly and can be used as a decision-making tool. In conclusion, this tool can be used to assist in designing distillation column system that will reduce negative impacts to the ecosystem.

However, there are still application limitations of this tool since the user needs to key in all the data manually into the tool. In the future, the tool will be further improved by automatically extracting all the required information from the process simulator. Furthermore, this tool can only performed sustainability analysis for a single distillation column system which can be used to test case studies from industry since it involves more than a unit distillation column in chemical processes. Therefore, it is encouraged that the tool can be upgraded to able to perform the sustainability analysis for multiple distillation columns.

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