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Pollution Prevention in Butyl Acetate Process Plant using WAR algorithm

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Abstract : This original research work objective is pollution prevention in butylacetate process plant using waste reduction algorithm (WAR). Butyl acetate process plant is designed using ASPEN PLUS V8.8. Potential environmental impacts (PEI) scores of all chemicals in the process are calculated using WAR algorithm. To minimize the pollution, process modification suggested is arranging recycle stream in the process. PEIs of modified process and the base case process were compared. Modified process was identified as the efficient process in minimizing the pollution. Economical and energy comparisons are also made for modified and base case processes. Utilities are reduced by 19% of the base process. Finally a plantwide control structure is developed to control the plant. From tuning tests it is identified that the developed control structure is good in controlling the process.
Key words : Plantwide control, Potential environmental impacts, WAR algorithm.

1. Introduction

The Waste Reduction algorithm (WAR) was developed by Environmental protection agency of United States scientists to evaluate environmental impacts of process designs [1,2]. WAR reduces environmental and related human health impacts at the design stage itself. WAR evaluates processes in terms of potential environmental impacts [3- 6].

Pollution prevention policies declare that pollution should be prevented or reduced at the source itself [7] or recycled in an environmentally safe manner [8, 9, 10]. Pollution prevention is a sustainable process development technique which lowers operating costs by utilizing resources effectively by reducing energy losses which decreases treatment and disposal costs [11, 12]. Sustainable process designs needs process modification methodologies for minimization of pollution or generation of waste [5, 13-18]. In open literature we can find various process modification methodologies to design sustainable processes [19-24]andeconomic processes [20, 25, 26]. These steps need the effective usage of process simulators [26, 27]. Systematic design procedures are needed for practicing engineers in industry to design sustainable processes to control generation of pollution or waste [3, 28-32]. Process integration is one of the techniques used to effective utilization of energy [33, 34].

Objectives of process industries are fulfilled by reducing the time required to get new products to market, increasing the quantity and quality of product produced, operating the plant more safely and efficiently [35] and by designing the plants for an optimum performance along their lifecycle. In literature several problems present in process industries and their remedial measures were discussed to improve the process performance [. For example plantwide control studies[36], azeotropic distillation column control [37], reactive distillation column control[38], dynamic modeling of process plants [39] and design and control of process plants [40, 41]. All these studies used ASPEN Dynamic plant simulation tool to address the environmental and economy of the process plants.

The objective of this work is to calculate potential environmental impacts of chemicals within the process at early stages of process design by using WAR algorithm. As a part of that to explain the application procedure, butylacetate production process was designed using ASPEN PLUS V8.8. WAR algorithm was applied to the butylacetate production process to suggest process modifications in such a way that, utilizing the resources effectively by minimizing the waste or pollution in industrial processes. Finally the designed process was controlled by designing a proper control structure using ASPEN DYNAMIC SIMULATOR V8.8.

2. Material and Methods

2.1 Materials

ASPEN PLUS V8.8 chemical process simulating tool was used to design the butylacetate process plant. Waste Reduction algorithm was used to calculate the potential environmental impacts (PEI). ASPEN DYNAMICS V8.8 simulating tool was used to design control structure to the process plant.

2.2 Methods

2.2.1 Steady state simulations

Process flowsheet was designed using ASPEN PLUS V8.8. Steady state simulations were performed for the designed flowsheet. The plant has two principal process unit operations: one continuous stirred tank reactor, three distillation columns. Two products are generated from the two reactants. The stoichiometry with reaction kinetics are:

$C_3H_6O_2 + C_4H_{10}O \rightarrow CH_4O + C_6H_{12}O_2$ (1)

$CH_4O + C_6H_{12}O_2 \rightarrow C_3H_6O_2 + C_4H_{10}O$ (2)

$R_1 = k_1 C_{C3H6O2} C_{C4H10O}$; $R_2 = k_2 C_{CH4O} C_{C6H12O2}$

$k_1 = 7 \times 10^6 e^{-71,960/RT}$; $k_2 = 9.467\times 10^6 e^{-72,670/RT}$

Figure 1 shows the process flow diagram for the base case process for the production of butyl acetate. Process contains one reactor for reaction and three distillation columns for the separation of products. ASPEN PLUS V8.8 process simulator was used for the process development.

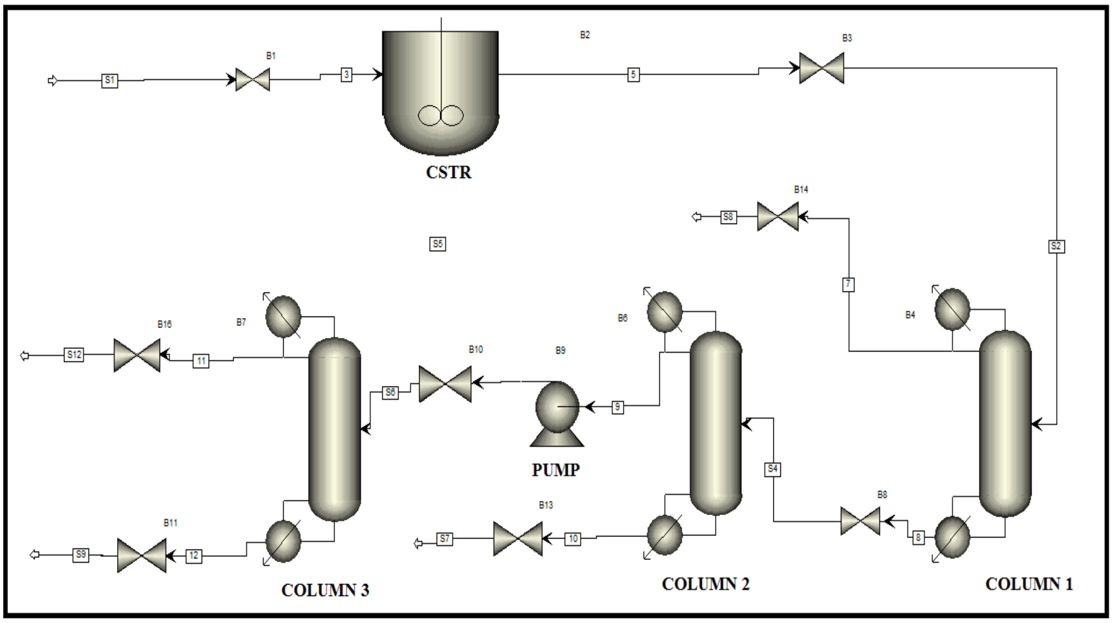

Figure 1. Base Case Process

2.2.2 Sensitivity Analysis

This study is used to study the effect of changes in input variables on process model outputs or to verify the feasibility of a solution to a design specification, for rudimentary optimization and to study the time varying variables using a quasi-steady state approach. Sensitivity analysis is carried out, to weigh the available options for reducing waste. Here reactor temperature was varied from 70^0C to 80^0C to know the variations in concentration of Butyl acetate in the reactor outlet stream for variation in reactor temperature. Results are shown in figure 2. Concentrations of butyl acetate steadily increased in the range of temperatures 70^0C to 80^0C.

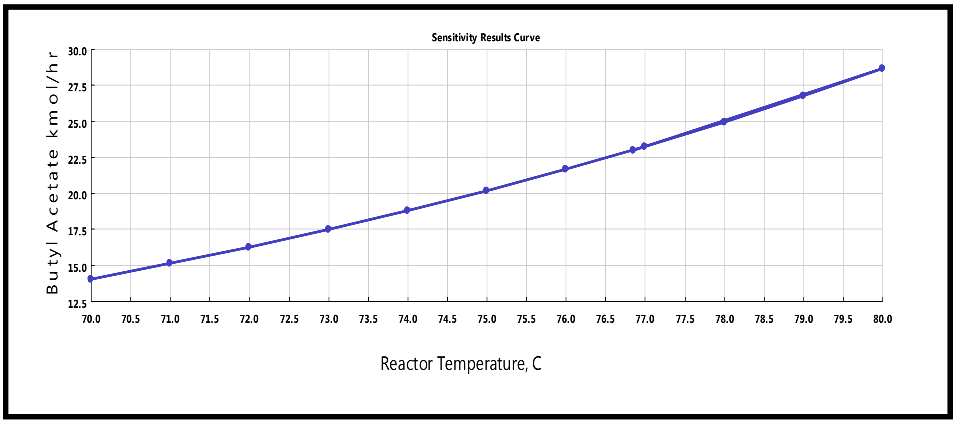

Figure 2. Sensitivity plot

2.2.3 Application of WAR algorithm

The WAR algorithm was reported in detail [42]. The same methodology is used here. WAR algorithm calculates Potential Environmental Impact (PEI) of a chemical. PEI is defined as its effect on the environment. Potential environmental indexes are: Human Toxicity Potential by Ingestion(HTPI), Human Toxicity Potential by Exposure(HTPE), Aquatic Toxicity Potential(ATP), Terrestrial Toxicity Potential(TTP), Global Warming Potential(GWP), Ozone Depletion Potential(ODP), Smog Formation Potential (PCOP), Acidification Potential(AP) [6].

WAR algorithm uses a process simulator and then calculates the pollution index of each stream. The design hierarchy for implementing waste minimization options is part of the process and it shown in the figure 3. Design hierarchy handles the low cost and technically easier tasks first. Sensitivity analysis determines the relative impact of various process modification options on pollution generation. The economic feasibility of introducing the best process modification option is studied before making the final decision. The WAR algorithm provides a systematic design procedure based on the pollution index of a product. ASPEN PLUS V8.8 process simulator is coupled with WAR to carry out material balance calculations for the butylacetate production process. From these results the pollution indices of the overall process and its different streams are computed. The economic feasibility of the selected process is then examined using ASPEN ECONOMIC ANALYZER V8.8. WAR algorithm identifies the process units that need to be considered for modification based on sensitivity analysis.

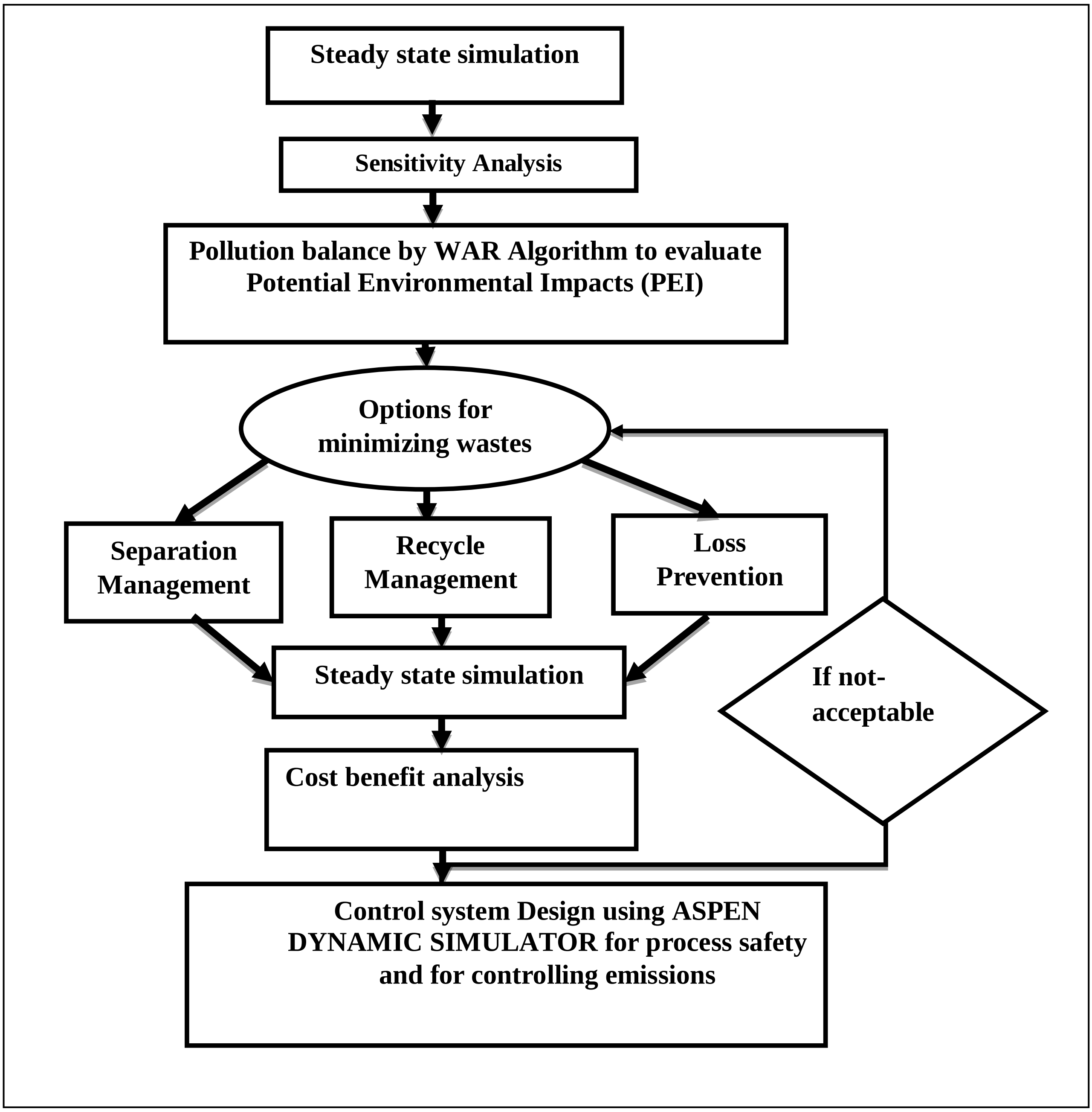

Figure 3: Design hierarchy for implementing waste minimization Options

Reports file was generated for the base case process shown in figure 1.The report file is used as input file for the WAR algorithm. WAR algorithm graphical user interface was shown in figure 4. The same procedure is applied to the modified process also shown in figure 5. WAR algorithm gives the pollution indexes of the streams and individual components in terms of graphs and tables.

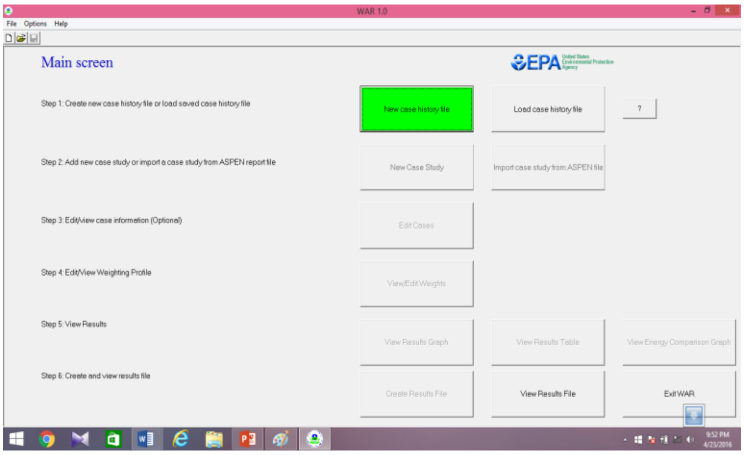

Figure 4. Graphical user interface of WAR algorithm

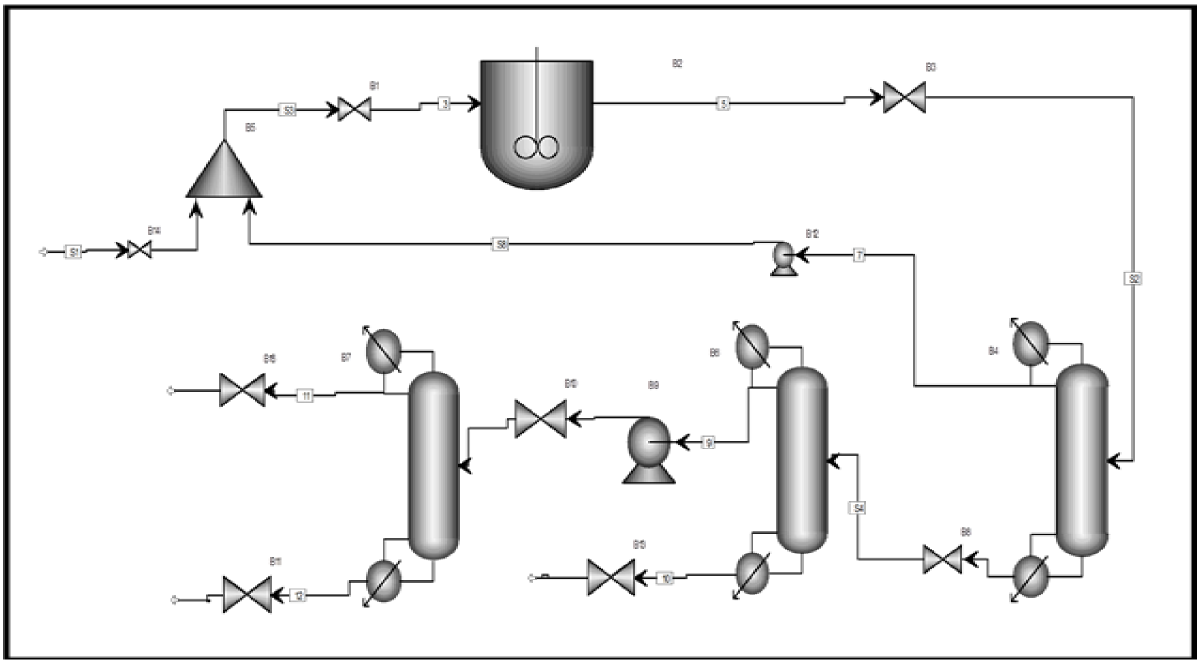

Figure 5. Modified Process

2.2.4 Dynamic Simulations

Once the steady state simulations were completed the steady state simulation flowsheet was inserted with control valves to complete the plumbing work. Pressure drops were verified such a way that fluid will pass easily through all the lines in the process flow sheet. The steady state simulation is converted in to ASPEN DYNAMICS. Sizing operations were completed for each block in the process. Control structure was designed and controller tuning performed. Finally the best operating conditions can be identified and they can be used in the final design of the process equipment.

2.2.5 Control structure design

Figure 6 shows the plantwide control structure for the butylacetate production plant. Before performing the dynamic simulations on the control structure, conventional PID controllers are arranged in all loops.

For CSTR: level controller and a temperature controller. For distillation column B4: one level controller at sump, one level controller at reflux drum and a pressure controller for reflux drum. For distillation column B6: one level controller at sump and a pressure controller for reflux drum. For distillation column B7: one level controller at sump, one level controller at reflux drum and a pressure controller for reflux drum were arranged.

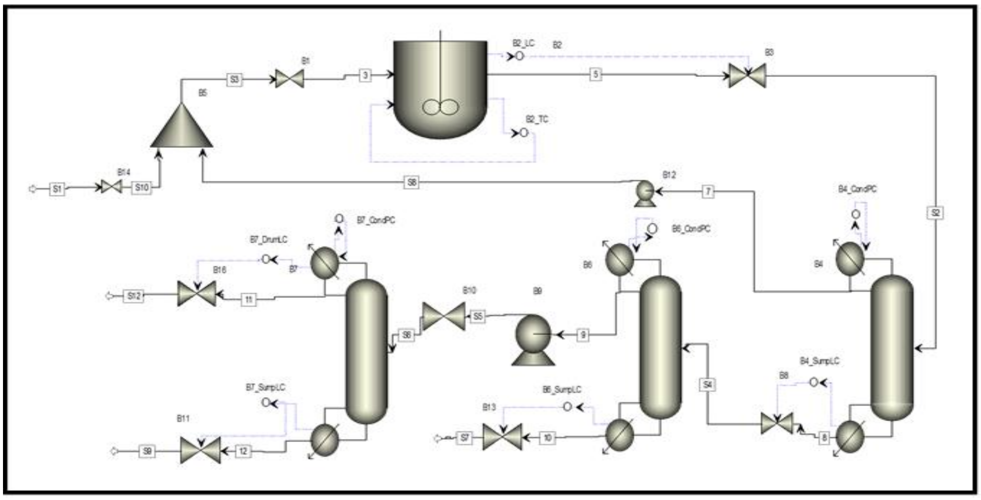

Figure 6. Process flowsheet for Butylacetate dynamic simulations

2.2.6. Controller design

Once the decentralized control structure was designed, dynamic simulations were performed using Aspen Dynamics. A third-order 0.5 min time lag was assumed for temperature measurement. Proportional-integral controllers were used for flow, pressure, composition, and temperature, level controls. Relay feedback tests were performed on the temperature loops to find the ultimate gain (Ku) and ultimate period (Pu) of each temperature control loop, and initial controller parameters were calculated according to Kc (Ku/3) and t_I (2Pu). In order to obtain an acceptable damping, further detuning from the initial settings.

3. Results and Discussion

3.1 Steady state simulations and WAR algorithm

Modified process was shown in figure 5. Potential environmental impact values for the base case process and for the modified process are shown in figure 7. Table 1 gives the extracted PEI values of the chemicals from the base case process. Table 2 gives the economic comparison of the base case process and the modified process. Modified process is more economical compared to the base case process and the modified process reduced the utilities by 19%. Table 3 gives the PEI values of both base case and modified processes. Same values are plotted in in Figure 7. It is evident that the total PEI value is low for the modified process and it generates less waste or less pollution compared to the base case process.

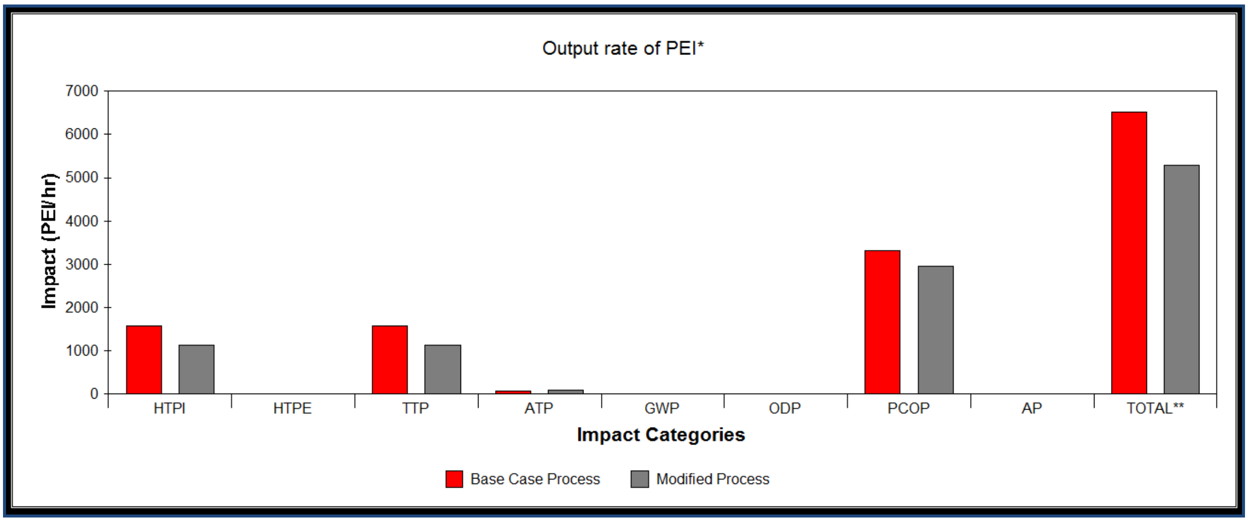

Figure 7. PEI plot

Table 1. The potential impact values (PEI) for each category of the chemicals in the process

Compound	HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP	Total
Methyl acetate	0.1122	0.0004	0.1122	0.0010	0.0000	0.0000	0.0216	0.0000	0.2474
Methanol	0.0667	0.0009	0.0667	0.0000	0.0000	0.0000	0.2122	0.0000	0.3465
Butyl Acetate	0.0267	0.0003	0.0267	0.0220	0.0000	0.0000	0.2514	0.0000	0.3271
1-Butanol	0.4756	0.0008	0.4756	0.0002	0.0000	0.0000	0.8959	0.0000	1.8481

Table 2. Economic benefits comparison between base case and modified process

Cost	Actual Process	Modified Process
Total Capital Cost [USD]	9363070	9090590
Total Operating Cost [USD/Year]	4477130	3954620
Total Utilities Cost [USD/Year]	2481050	2010390
Equipment Cost [USD]	1373400	1289400
Total Installed Cost [USD]	3162100	2950300

Table 3. Total output rate of PEI (PEI/hr)

Case	HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP	TOTAL
Base Case	1.57E+03	4.24E+00	1.57E+03	6.05E+01	0	0	3.31E+03	0	6.51E+03
Modified process	1.13E+03	4.01E+00	1.13E+03	8.88E+01	0	0	2.95E+03	0	5.29E+03

3.2 Dynamic simulations

3.2.1 Pressure controllers

Plantwide control structure developed for the overall plant is shown in figure 6. Controller face plates are shown in figure 8. Pressure controller tuning constants are a gain of 20 and integral time of 12 min.

3.2.2 Level controllers

There are totally six level controllers arranged for the reactor and three distillation columns. All level loops are proportional with K_C = 10 and integral time of 60 min. For reactor one level controller is arranged with direct reverse controller action.

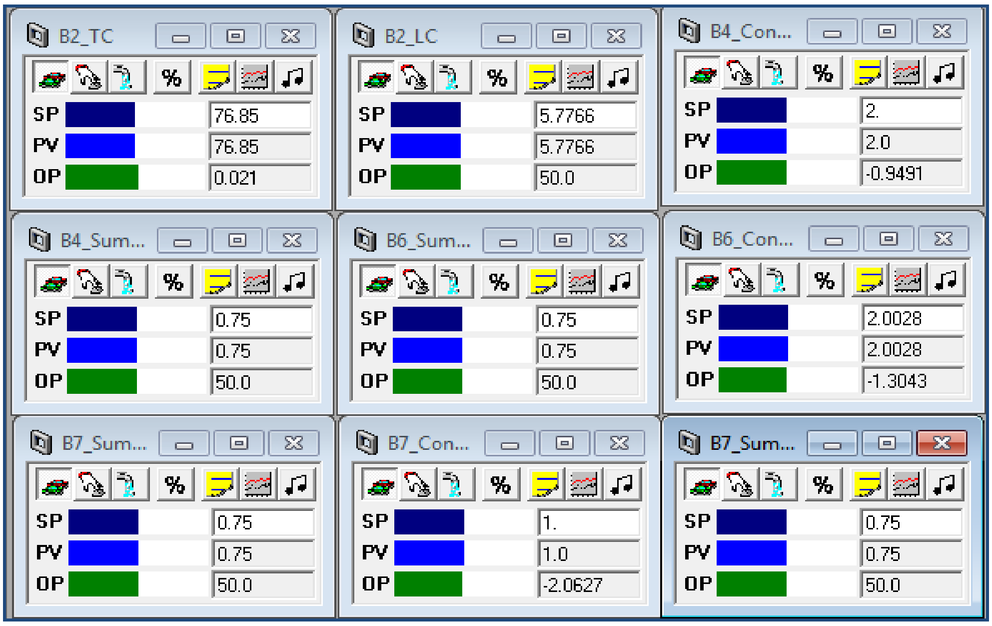

Figure 8. Controller faceplates

3.2.3 Reactor temperature control

The steady state time was reported as 5.6 hours. Temperature controller controller initial output is 0.016946 MMkcal/hr, gain 5 and integral time constant 6 min. controller action is reverse. Then closed loop ATV test is performed. The default value of the relay output amplitude is 5%, which is usually good.

3.2.4 Performance Evaluation

For disturbances the performance is evaluated from transient response plots. For CSTR temperature controller ultimate gain is 69.5, ultimate perid is 54.6 min. Tyreus luyben values are ultimate gain 100 and ultimate period 1.8 min. Tuning parameters are gain 31.3487 and integral time 3.96 min.

4. Conclusions

This work discussed the application of the waste reduction (WAR) algorithm to butyl acetate process plant. The procedure developed in this work can be generalized to various industrial processes. This process explained design alternatives to effective utilization of resources by minimizing the wastes or industrial pollution. Dynamic simulations were performed for total process plant. Modified process saved 19% of the utility cost compared to the base case process. Modified process is safe to environment and it is more economical compared to the base case process.

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