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COWAR: A CAPE OPEN Software Module for the Evaluation of Process Sustainability

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The sustainability of a chemical process can be estimated using qualitative and quantitative indicators. Quantitative indicators, such as potential environmental impact (PEI) indexes, are essential for evaluating the environmental impact of a chemical process and for choosing the best design among available alternatives. Waste Reduction (WAR) Algorithm, used to calculate the PEI indexes, is implemented using a standard methodology, CAPE OPEN (CO). Such development leads to COWAR, a software module for the evaluation of process sustainability. Details regarding the COWAR development and function are presented in this work. Finally, a representative chemical process is presented to demonstrate the software applicability. © 2008 American Institute of Chemical Engineers Environ Prog, 27: 373–382, 2008

Keywords: WAR algorithm, CAPE OPEN, sustainability, process simulation, decision-support systems

INTRODUCTION

Sustainability is an important social, political, and scientific issue of this century. Chemical companies are involved in various activities aimed at addressing sustainable development. Sustainable development has been defined as the creation of goods and services using processes and systems that are nonpolluting; conserving energy and natural resources; economically viable; safe and healthy for employees, communities and consumers; socially and creatively rewarding for all working people [1]. In practical terms, industrial sustainability means employing technologies and know-how to use less material and energy, maximizing renewable resources as inputs, minimizing generation of pollutants or harmful waste during product manufacturing and use, and producing recyclable or biodegradable products [2].

Economy, society, and environment are three basic elements of sustainability. This work addresses mainly the environmental pillar, with the detailed analysis of the impact to the environment of the emissions. Nonetheless, since it also considers the energy consumption of the process under study, it partly addresses the economic issues of the sustainability, even if a more complete treatment will be necessary. Social concerns of chemical processes are outside the scope of this work.

To eliminate or reduce negative environmental problems, the environmental performance of chemical processes should be identified and quantified at an early stage of process design. The quantitative analysis of environmental performance of alternative processes is an ongoing task and remains a controversial topic. Although various methods are available in the literature, a generalized method has not been established yet [3]. Some of these methods are: Waste Reduction (WAR) Algorithm, Process Environmental Performance Assessment (PEPA), and Global Environmental Risk Assessment (GERA) [3, 4]. In this article, WAR Algorithm is used for the development of a software module based on the CAPE OPEN (CO) technology. The choice of the CAPE OPEN technology has been made according to a precise goal: to develop a module able to interact with all the process

simulator software programs which support the CO interfaces. Once the module is created it is ready to be used anywhere, being independent of the process simulator software used. This is one of the greatest advantages offered by the CO technology.

GENERAL DESCRIPTION OF THE WAR ALGORITHM AND PEI

The WAR Algorithm, proposed by Cabezas, is based on potential environmental impact balance, analogous to mass or energy balances [5–7]. The overall impact balance for a general chemical process contains the impact generated by the chemical process and the impact generated by the energy generation process linked to the chemical process. This information is used for the calculation of environmental indexes, which characterize the relative environmental efficiency of the process. There are two different index classes: indexes associated with potential environmental impact output; and indexes associated with potential environmental impact generation. Among output indexes, the two most important ones are: the total rate of impact output, $\dot{I}_{out}^{(t)}$ and the total impact output per mass of products, $\hat{I}_{out}^{(t)}$. Among generation indexes, the two most important ones are: the total rate of impact generation, $\dot{I}_{gen}^{(t)}$; and the total impact generated per mass of product, $\hat{I}_{gen}^{(t)}$ defined. These indexes are calculated using the results of process simulators (mass flow-rates and composition of the process input, output and waste streams) and the toxicological data for the substances involved in the process.

IMPLEMENTATION OF THE WAR ALGORITHM IN PROCESS SIMULATORS—CAPE OPEN METHODOLOGY

General Information on the CAPE OPEN Methodology

Process industries are facing increasing economic, environmental and safety constraints and are being forced to improve the performance of their plants by reducing the costs of, and time required for, plant and product development. Simulation software, specific to process industries, provides a vital tool for achieving these goals and being competitive on a market with increasingly short innovation cycles. CAPE (Computer Aided Process Engineering) is progressively more required by process industries. A standard to allow communication between CAPE software components from different sources (software and equipment vendors, universities, and in-house) constitutes one of the ways to provide process industries with faster, cheaper, more accurate process simulation, leading to enhanced competitive and environmental performance [8]. With this goal in mind, the CAPE OPEN project has been created.

CAPE OPEN (CO) is a cooperation project aimed at defining software interfaces for plug-and-play simulation components for the various process simulators on the market. The CO idea is to develop a standard way of representing a process, its chemical components, unit operations and connectivity. CO objectives are to enable native components of a simulator to be replaced by those from another independent source or from another simulator with minimum effort, in as seamless a manner as possible [9]. In other words, once the components are developed, they are available for use anywhere. The integration of the different computational components is performed by the standard CO interfaces, in other words the components are able to "talk to each other" via defined interfaces. The CAPE-OPEN Interface System architecture is based on an object-oriented technology, which allows software systems to be constructed from binary software components. The job of the interface is to translate requests for information or action, by either part, into something the other understands (CAPE OPEN Open Interface Specifications Unit Operations, 1999).

Today, there are a number of process simulators, such as AspenTech simulation products (Aspen Plus and Aspen Hysys), Invensys simulation products (PROII), AmsterChem simulation product (COCO/COFE software, Process Systems Enterprise simulation products (gPROMS), Honeywell Process Solutions (UniSim Design), ProSimPlus (ProSim SA) which interface software components.

IMPLEMENTATION OF THE WAR ALGORITHM USING THE CAPE OPEN METHODOLOGY

A process simulator should be used to obtain environmental information during the process design phase. The goal is to evaluate the friendliness or unfriendliness of a chemical process, independently of the process simulator used. In this context, the equations of the WAR Algorithm have been implemented in a CAPE OPEN unit operation, which is part of the software module COWAR. The equations of the WAR Algorithm, present in the literature [5–7], are reported in Appendix.

The "unit operation" is a well-known concept for chemical engineers. Some specific elements and the understanding of their meaning are requested in order to develop a unit operation (UO) model using the CO technology (e.g. a heat exchanger, a reactor, a mixer, a splitter, a distillation column, etc.) These elements are explained in the next section.

For each UO developed in CO the concepts "stream" and "port" should be marked out. These elements are defined in the "specification" step of the UO development and represent indispensable elements for the CO unit operation. The "stream" concept is used to describe different internal representations that simulators use to record the different types of flows that exist in the physical processes. Streams are divided into material streams, energy streams and information streams. The "ports" concept is used to represent a software interface that enables contents of the proprietary simulator streams to be accessed. Ports provide a standard way to fetch data from the simulator executive and to return data to the simulator executive [10]. The ports are characterized by the following elements: name, description, direction, and the port type. For example for a distillation column the names of the ports could be: "column feed," "top product," "bottom product," "reflux ratio," or for a mixer the ports could be: "input1,"

Table 1. Values assumed by the COWAR parameters.

Chemical process		Energy generation process	
Name of the parameter	**Value**	**Name of the parameter**	**Value**
Process type	0	Process type	1
CO position	0 (for the input stream) 1 (for the waste stream) 2 (for the output-product-stream) 3 (for the internal stream of chemical process)	CO position	0 (for the input stream) 1 (for the waste stream)
CO name	0 1 . N-number of CO modules inserted in the process	CO name	0 1 . N-number of CO modules inserted in the process

"input2," ..., "input n," "output1," "output2,"..., "output n". Any name can be chosen for the name of the ports. A brief description of the ports could also be provided in the "description" section. The port has also a direction which can be inlet or outlet. The direction attribute defines whether a port delivers information to a UO (input port) or receives information from a UO model (output port) (Conceptual Design Document, CAPE OPEN Team, 2000). The type of connections (material, heat or work) should be also specified. The three ports type corresponding to the three classes of information are Material Port, Energy Port, and Information Port. The material port is the most common one. It should be also specified that any number of input or output ports can be defined. The ports will be used in the process simulator for connecting the process simulator streams with the CO Module. UO modules can also have sets of parameters (these are optional elements). The "parameters" concept represents information that is not associated with the ports, but that the modules wish to expose to their clients. Typical examples include equipment design parameters (e.g. the geometry of a reactor, pressure drop for a valve, outlet hot temperature for a heat exchanger), and important quantities computed by the module (e.g. the capital and operating cost of a reactor) [11].

Based on the above presented theory the COWAR module is exemplified below.

The CAPE OPEN UO, COWAR, was built using the CAPE OPEN Unit Wizard 0.9.3 and later the COWAR has been modified to be compatible with the new wizard version CAPE OPEN Unit Wizard (version 1.0). The CAPE OPEN Unit Wizard is available on CAPE OPEN Laboratories Network CO-LaN website (**www.colan.org**).

The COWAR module contains a UO which has one input port, one output port and three parameters. The process type, position and name of the CO UO were defined as real parameters. With regard to the necessity of using three parameters, it should be specified that: the process type parameter is used to identify the type of process (chemical or energy generation process); the position parameter is needed for the location detection of the CO in the flow sheet (the CO could be on an input, output, intermediary, or waste stream of the process); and the name parameter is needed to find the CO units which were first classified using the position parameter. The values assumed by the parameters are presented in Table 1.

As it has been mentioned before, the creation of COWAR has been facilitated by a wizard, available on the CO-LaN web site (**www.colan.org**). The CAPE OPEN Unit Wizard does not generate all the code needed for a complete UO. In this regard, the ICapeUnit_Calculate subroutine of the Visual Basic code should be modified. This is the place where the equations of the WAR Algorithm (see Appendix) have been implemented. The ICapeUnit_Calculate subroutine is also connected to a database [of the Environmental Protection Agency (EPA)], which contains the Environmental Impact Categories for more then 1700 substances. The connection between the CO Module and the database is done by using ADO (ActiveX Data Objects) technology. The COWAR Module is able to attribute the input stream properties to the output stream. In other words, the output stream is equal to the input stream (flow-rate, temperature, pressure, composition). The subroutine reads from the database the normalized values for the environmental impact categories of the substances involved in the chemical process. The Environmental Impact Indexes ($I_{out}^{(t)}$, $\hat{I}_{out}^{(t)}$, $I_{gen}^{(t)}$, and $\hat{I}_{gen}^{(t)}$) are calculated using the PEI balance equations around the chemical process and the energy. The schema containing the main steps, tools and expected results of the methodology described above is presented in Table 2.

IMPACT CATEGORIES DATABASE AND ITS CONNECTION WITH COWAR

As mentioned in the previous section, in order to calculate the Environmental Indexes, the Environmental Impact Categories are requested. The WAR Algorithm uses eight environmental impact categories

Table 2. The implementation of the WAR in a CAPE OPEN unit operation.

	Steps	Tools	Results
1. Development of CO Unit Operation	1.1. Build the CO Unit Operation	CAPE-OPEN Unit Wizard	CO Unit Operation
	1.2. Modify the ICapeUnit_ Calculate	VB, EPA Data Base	CO Unit Operation with WAR Algorithm
	1.3. Build the dll	VB	dll of CO
	1.4. Install the dll	VB	CO installed
	1.5. Test the CO Unit Operation	CAPE Tester	CO tested
2. Development of the process flow-sheet	2.1. Design the flow-sheet	Process Simulator	The flow-sheet of the chemical process
	2.2. Define the components	Process Simulator	The flow-sheet of the chemical process
	2.3. Define the thermodynamic method	Process Simulator	The flow-sheet of the chemical process
	2.4. Define the streams	Process Simulator	The flow-sheet of the chemical process
	2.5. Define the units operation	Process Simulator	The flow-sheet of the chemical process
	2.6. Design specifications	Process Simulator	The flow-sheet of the chemical process
3. Calculation of the chemical process impact Calculation of the energy generation process impact	3.1. Recognize the CO Unit Operation in process simulator	Process Simulator	CO Unit Operation recognized in the process simulator
	3.2. Insert the CO Unit Operation in the chemical process flow-sheet	Process Simulator	Process flow-sheet for the chemical process with CO Modules
	3.3. Run the simulation	Process Simulator	The convergence of chemical process flow-sheet
	3.4. Insert the CO Unit Operation in the energy generation process flow-sheet	Process Simulator	The flow-sheet of the energy process
	3.5. Run the simulation	Process Simulator	The convergence of the energy process

in its evaluation. The categories are the following [7]: Human Toxicity Potential by Ingestion (HTPI); Human Toxicity Potential by Exposure (HTPE); Terrestrial Toxicity Potential (TTP); Aquatic Toxicity Potential (ATP); Global Warming Potential (GWP); Ozone Depletion Potential (ODP); Photochemical Oxidation Potential (PCOP); and Acidification Potential (AP).

These impact categories values are taken from a database and used to calculate the environmental impact through PEI indexes. The most complete database, which contains all eight Environmental Impact Categories needed for the implementation of the WAR Algorithm, is the Environmental Protection Agency database (DB). In the ICapeUnit Calculation subroutine of the CO Unit Operation developed (COWAR), there is a module which makes the connection between the process simulator and the EPA DB. The CO reads the composition (mass fraction) of each stream. The composition leads to the CAS-Number of substances present in the stream. The normalized values of the impact categories are read as a function of the CAS-Number and then used in the calculation of PEI Indexes. The procedure is summarized in Figure 1. It should be also specified that the normalization of impact categories is necessary to: ensure that values of different categories contain the same units to allow their combination for the calculation of the overall potential environmental impact; and ensure that values from different categories have, on average, equivalent scores [6].

DISCUSSIONS ON THE WEIGHTING FACTORS OF THE ENVIRONMENTAL IMPACT CATEGORIES

According to Young and Cabezas, the overall potential environmental impact of chemical k, ψ_k, can be determined by summing up the specific potential environmental impact of chemical k, ψ^s_{kl}, on all of the possible impact categories:

$$\psi_k = \sum_l \alpha_l \psi^s_{kl}$$

where α_1 represents the relative weighting factor of impact category l [6].

The weighting factors are essential for WAR Algorithm because they permit the combination of the

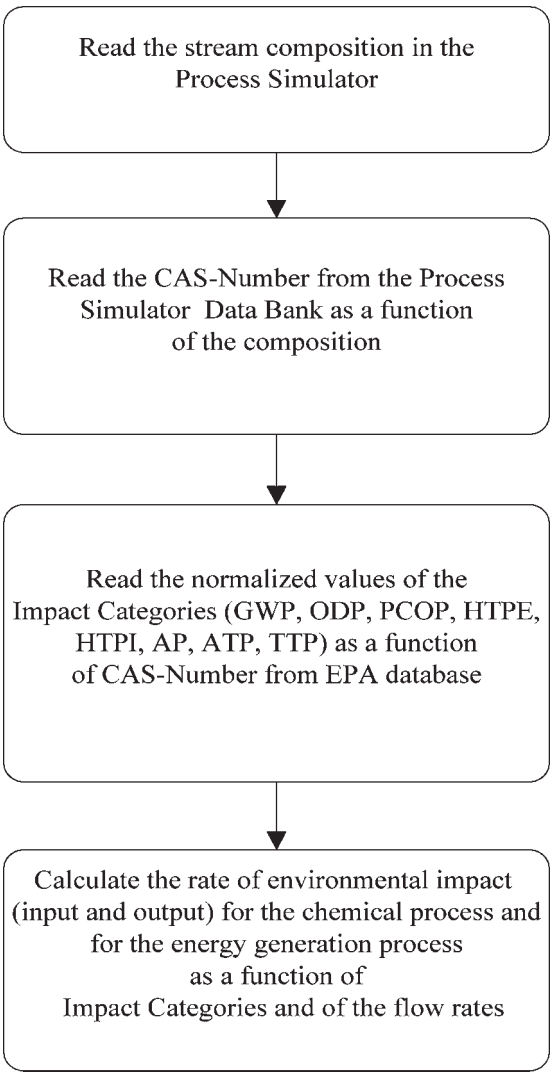

Figure 1. The connection between CO Unit Operation and EPA's database.

impact categories according to local needs and policies. One modification on the weighting factors of the environmental impact categories will affect the final PEI (see the equations for Appendix). Obviously, the comparison among different process alternatives in terms of potential environmental indexes should be done with the same weighting factors. It should be also underlined that, in the case studies analyzed using the COWAR Module, the weighting factors have been considered equal to unity. This is a reasonable way of thinking in order to calculate the maximum potential environmental impact. If there are some realistic reasons (e.g. local needs) to consider the weighting factors lower then one, then the potential environmental impact will be calculated with these specific values of the weighting factors. Anyway, unitary values of the weighting factors should be taken into account as references values for making the comparison between the highest potential environmental impact (obtained with unitary values for the weighting factors) and the potential environmental impact calculated using weighting factors lower then one.

CASE STUDY EXAMPLE: PHTHALIC ANHYDRIDE PRODUCTION

The methodology described was applied in the phthalic anhydride production process.

GENERAL INFORMATION

The methodology described above was applied in the case study of phthalic anhydride production. Two case studies: the production of phthalic anhydride by oxidation of o-xylene and production of phthalic anhydride by oxidation of naphthalene, have been considered, simulated and compared in terms of sustainability.

PROCESS DESCRIPTION

Process schema for the production of phthalic anhydride by oxidation of o-xylene is presented in Figure 2. The raw materials are air and o-xylene. The hot air and vaporized o-xylene are mixed and sent to a packed bed reactor where the following reactions occur:

$$\underset{\text{o-xylene}}{C_8H_{10}} + 3\ O_2 \rightarrow \underset{\text{phthalic anhydryde}}{C_8H_4O_3} + 3\ H_2O$$

$$\underset{\text{o-xylene}}{C_8H_{10}} + 7.5\ O_2 \rightarrow \underset{\text{maleic anhydryde}}{C_4H_2O_3} + 4\ H_2O + 4\ CO_2$$

$$C_8H_{10} + 11.5\ O_2 \rightarrow 8\ CO_2 + 5\ H_2O$$

$$C_8H_{10} + 6.5\ O_2 \rightarrow 8\ CO + 5\ H_2O$$

After the reactions, the products and by-products are sent to a flash, where the gaseous phase is separated from the liquid phase. The gaseous phase contains carbon dioxide, carbon monoxide, unreacted oxygen, nitrogen, and water. The next step is the separation of the liquid phase which occurs in two distillation columns. The first distillation column separates the o-xylene from the phthalic anhydride and maleic anhydride. The recovered o-xylene is recycled. The goal of the second column is to separate the phthalic anidryde (the product of the process) from the maleic anhydride (by-product). The product must have a purity of 99.9% in phthalic anhydride [12].

Another way for obtaining phthalic anhydride is by using naphthalene as the raw material. Process schema for the production of phthalic anhydride by oxidation of naphthalene is presented in Figure 3. The input streams are naphthalene and air feed. The naphthalene feed is heated and mixed with the air stream which is compressed and heated before being mixed with the naphthalene feed. The feed of the mixer is sent to the reactor, where the following reactions occur:

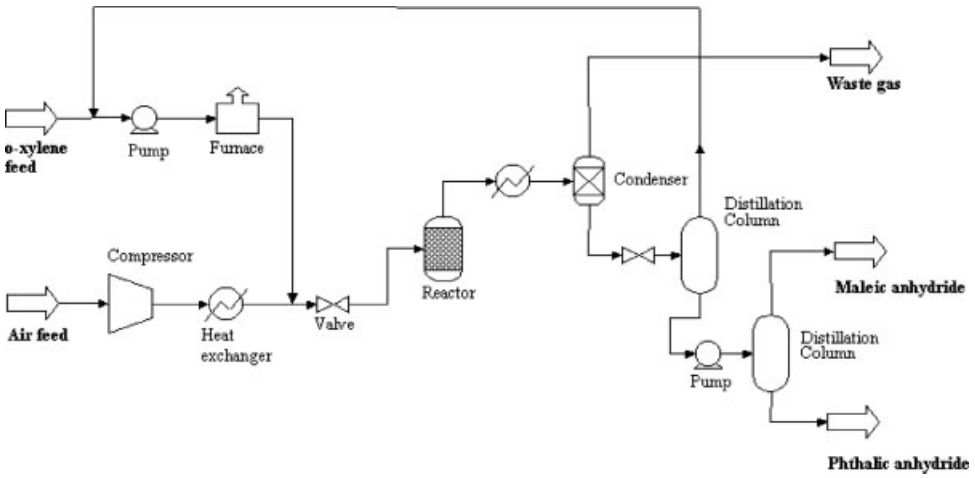

Figure 2. Production of phthalic anhydride from o-xylene.

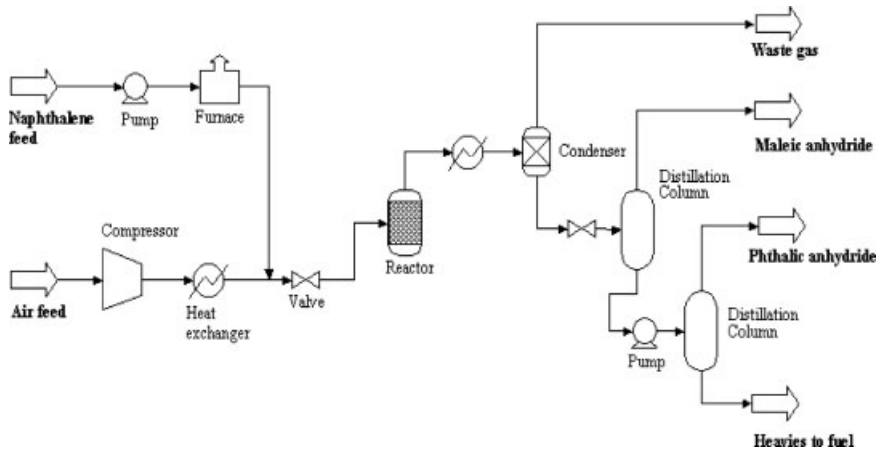

Figure 3. Production of phthalic anhydride from naphthalene.

$$C_{10}H_8 + \frac{9}{2}\ O_2 \rightarrow \underset{\text{phthalic anhydride}}{C_8H_4O_3} + 2\ H_2O + 2\ CO_2$$

$$C_{10}H_8 + 6\ O_2 \rightarrow 2\ \underset{\text{maleic anhydride}}{C_4H_2O_3} + 2\ H_2O + 2\ CO_2$$

$$C_{10}H_8 + \frac{3}{2}\ O_2 \rightarrow \underset{\text{naphthoquinone}}{C_{10}H_6O_2} + H_2O$$

$$C_{10}H_8 + 12\ O_2 \rightarrow 4\ H_2O + 10\ CO_2$$

$$C_{10}H_8 + 7\ O_2 \rightarrow 4\ H_2O + 10\ CO$$

The liquid phase is separated from the gas phase in a separator. After the separation, the liquid containing phthalic anhydride, maleic anhydride, and heavy fuel is sent to the separation part of the plant, which contains two distillation columns. In the first distillation column the maleic anhydride (a by-product) is separated in the top of the column. The second column has the role of separating the phthalic anhydride (main product of the process) from the heavy fuel (by-product).

PROCESS SIMULATION AND RESULTS

The processes were simulated using two process simulators (Aspen Plus and PROII). The goal of the simulations is to choose, from these two cases, the best environmental solution. The specifications of the input streams are presented in Table 3 and those of the output streams in Table 4. Table 5 contains the potential environmental impacts for the chemicals used in the process starting from o-xylene. The tables related to the production of phthalic anhydride, starting from naphthalene, are: Table 6, containing the input streams of the process; Table 7, containing the output streams of the process; and Table 8, contain-

Table 3. The specifications for the input streams of the phthalic anhydride process from o-xylene.

Name of the stream	Flow rate (kg/h)	PEI/h
o-xylene	10469	16554.2
Air	63967	0

Table 4. The specifications for the output streams of phthalic anhydride process from o-xylene.

Name of the stream	Flow rate (kg/h)	PEI/h
Off-gas	63219	332.65
Maleic anhydride	890.73	1040.90
Phthalic anhydride	10315.25	1255.37

Table 5. PEI of the substance used in phthalic anhydride process from o-xylene process.

Substance name	PEI (impact/kg)
o-xylene	1.58126
Oxygen	0
Nitrogen	0
Carbon dioxide	0.03795
Water	0
Maleic anhydride	1.18005
Phthalic anhydride	0.12170
Carbon monoxide	0.06538

Table 6. The specifications for the input streams of phthalic anhydride process from naphthalene.

Name of the stream	Flow rate (kg/h)	PEI/h
Naphthalene	12817.5	1162.47
Air	144250	0

Table 7. The specifications for the output streams of phthalic anhydride process from naphthalene.

Name of the stream	Flow rate (kg/h)	PEI/h
Off-gas	144760.52	602.97
Maleic anhydride	1569.19	1850.04
Heavies to fuel	150.16	1652.43

Table 8. PEI of the substance used in phthalic anhydride process from naphthalene.

Substance name	PEI (impact/kg)
Naphtalene	0.8708
Phthalic anhydride	0.1217
Maleic anhydride	1.1800
Naphthoquinone	5.4800
Oxygen	0
Water	0
Carbon dioxide	0.03795
Carbon monoxide	0.06554
Nitrogen	0

ing the potential environmental impacts. The data for the potential environmental impact of chemicals involved in the process proceed from the EPA DB (the sum of the normalized values of the impact categories). The potential environmental impacts were calculated using unitary weighting factors. The CO Unit Operation was directly incorporated in the process flow-sheet. The potential environmental impact input $\dot{I}_{in}^{(cp)}$ and the potential environmental impact output $\dot{I}_{out}^{(cp)}$ of the chemical process were calculated using the mass flow-rates of the chemical process input and output streams; the composition (mass fraction) of the chemical process input and output streams; and the normalized values of the PEI for each substance involved in the streams. The energy necessary for the chemical process was used to calculate the coal quantity burned in the energy generation process. Using the same procedure, the potential environmental impact input $\dot{I}_{in}^{(ep)}$ and the potential environmental impact output $\dot{I}_{out}^{(ep)}$ of the energy generation process were calculated. All these terms ($\dot{I}_{in}^{(cp)}, \dot{I}_{out}^{(cp)}, \dot{I}_{in}^{(ep)}, \dot{I}_{out}^{(ep)}$) were used in the calculation of the environmental indexes ($\dot{I}_{out}^{(t)}, \hat{I}_{out}^{(t)}, \dot{I}_{gen}^{(t)}, \hat{I}_{gen}^{(t)}$). The indexes were calculated in the same way for each case. The lower the value of these indexes the higher the environmental efficiency of a process. The design of the processes with lower environmental indexes needs to be constrained by economic and social considerations. The results are presented in Figures 4-7.

From the graphs presented, it can be noticed that the best environmental solution for phthalic anhydride production is case 1. The economical concerns should be also considered in choosing the best option. The productivity values for phthalic anhydride in the two cases are close (69.64 kmol/h for the o-xylene process and 69.89 kmol/h for the naphthalene process). The difference in productivity terms is very low (69.64 kmol/h vs. 69.89 kmol/h). The quantity of energy, which has to be supplied from external sources, is 61.52 BTU/h in the first case study and 33.14 BTU/h in the second case study. The chemical plants for the two processes are different, as it can be noticed from Figures 2 and 3, so the operating costs, directly linked with the energy consumption are different. The economical concerns support more the second alternative design as the best solution but from environmental sustainability point of view the choice of the first case is emphasized. This example is quite relevant to demonstrate that sometimes the environmental optimum does not coincide with the economical one.

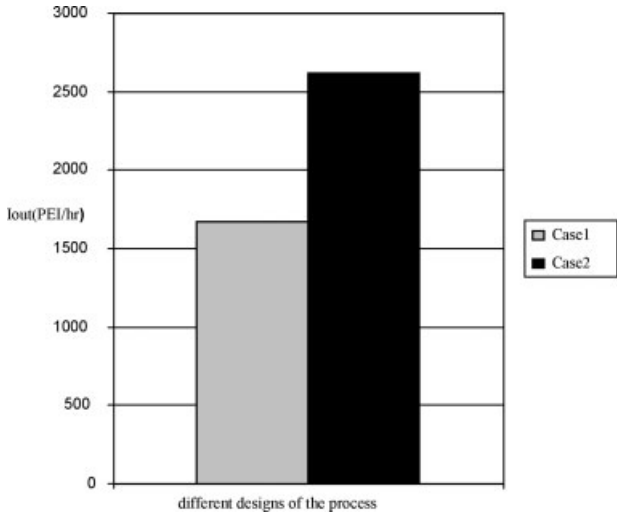

Figure 4. Iout (PEI/hr) for Phthalic Anhydride.

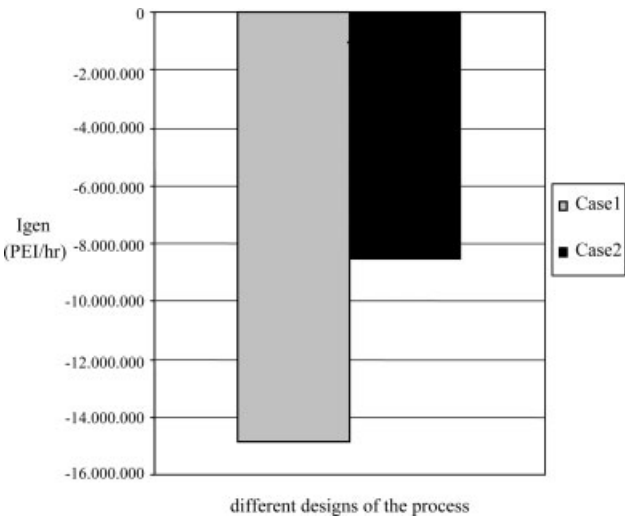

Figure 6. Igen (PEI/kg) for Phthalic Anhydride.

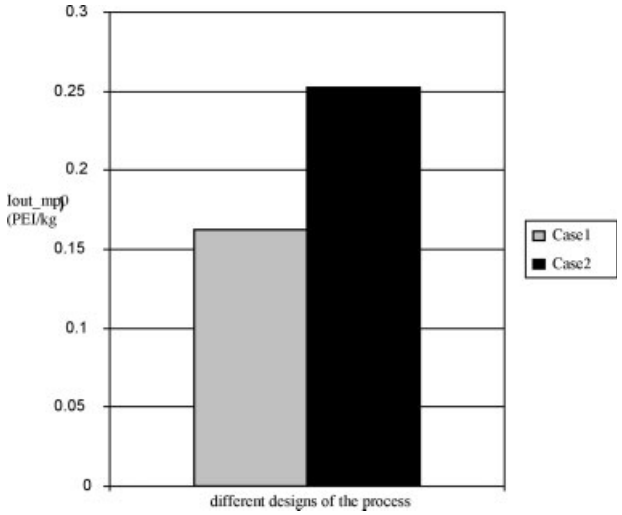

Figure 5. Iout_mp (PEI/kg) for Phthalic Anhydride.

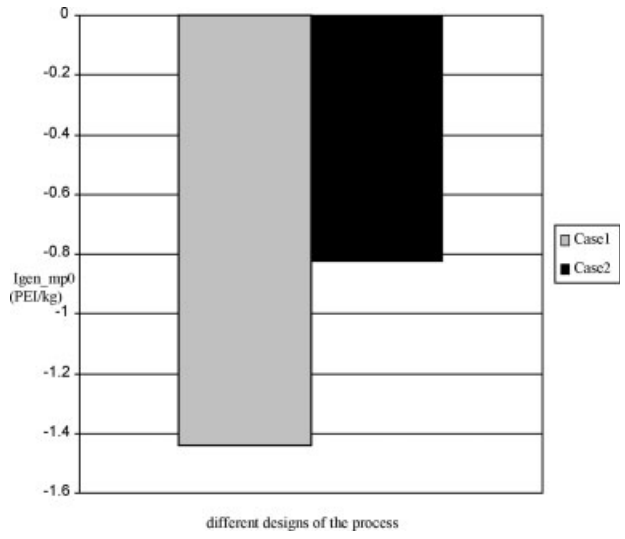

Figure 7. Igen-mp (PEI/kg) for Phthalic Anhydride.

CONCLUSIONS

The goal of this work was to develop a methodology for the implementation of WAR Algorithm, including the calculation of PEI Indexes, within the process simulation software, by using a standard interface (CAPE OPEN). This tool, COWAR, is a valid one used to select the best environmental process design for a chemical plant. The methodology was applied to several processes. The phthalic anhydride production is reported in the present article. In the case study presented, the product obtained was the same, even if two different options were evaluated (starting from o-xylene as raw material and naphthalene as raw material). The results obtained using the standard CAPE OPEN methodology applied to process simulators permitted the choice of the best design option. Considering the results reported in this article, the availability of the standard CO module (COWAR) directly interfaced with the toxicological data bank can be considered a powerful, reliable and easy-to-use method to help engineers in deciding on the sustainability of an industrial process at the design stage.

Future work will be focused on the estimation of impact categories for substances which are not included in the database and the tool chosen for this objective is molecular modeling.

The software module developed is available from the authors, upon request.

APPENDIX

The overall balances for a general chemical process, including also the energy generation facility, are illustrated in Figure A1.

The key element of the assessment involves a balance equation which has the following form:

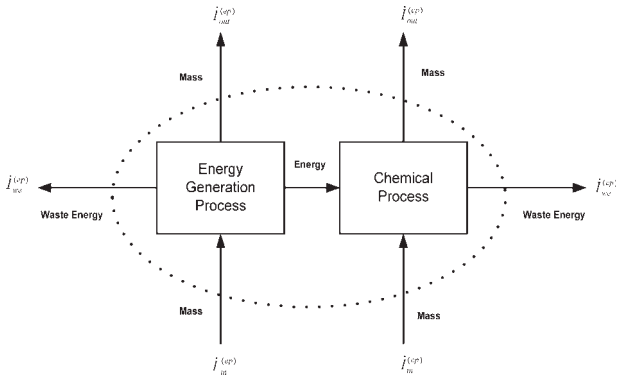

Figure A1. The overall environmental balances around a chemical process including the energy generation facility.

$$\frac{\partial I_{\text{syst}}}{\partial t} = \dot{I}_{\text{in}}^{(\text{cp})} + \dot{I}_{\text{in}}^{(\text{ep})} - \dot{I}_{\text{out}}^{(\text{cp})} - \dot{I}_{\text{out}}^{(\text{ep})} - \dot{I}_{\text{we}}^{(\text{cp})} - \dot{I}_{\text{we}}^{(\text{ep})} + \dot{I}_{\text{gen}}^{\text{syst}} \tag{A1}$$

I_{syst} is the amount of potential environmental impact inside the system; $\dot{I}_{\text{in}}^{(\text{cp})}$ and $\dot{I}_{\text{out}}^{(\text{cp})}$ are the input and output rates of potential environmental impact to the chemical process; $\dot{I}_{\text{in}}^{(\text{ep})}$ and $\dot{I}_{\text{out}}^{(\text{ep})}$ are the input and output rate of potential environmental impact to the energy generation process; $\dot{I}_{\text{gen}}^{\text{syst}}$ is the rate of generation of potential environmental impact inside the system; $\dot{I}_{\text{we}}^{(\text{cp})}$ is the rate of potential environmental impact output due to the emission from the chemical process [6].The expressions for the chemical process are:

$$\dot{I}_{\text{in}}^{(\text{cp})} = \sum_{j}^{\text{cp}} \dot{I}_j^{(\text{in})} = \sum_{j}^{\text{cp}} \dot{M}_j^{(\text{in})} \sum_{k} x_{kj}\, \psi_k + \ldots \tag{A2}$$

$$\dot{I}_{\text{out}}^{(\text{cp})} = \sum_{j}^{\text{cp}} \dot{I}_j^{(\text{out})} = \sum_{j}^{\text{cp}} \dot{M}_j^{(\text{out})} \sum_{k} x_{kj}\, \psi_k + \ldots \tag{A3}$$

$$\dot{I}_{\text{we}}^{(\text{cp})} = \sum_{j}^{\text{cp}} \dot{E}_j^{(\text{cp})} \psi x_{\text{we}} \approx 0 \tag{A4}$$

where $\dot{I}_i^{(\text{cp})}$ is the potential environmental impact input (i = in) or output (i = out) of the chemical process; $\dot{I}_j^{(i)}$ is the potential environmental impact flow rate with the stream j which may be an input or an output stream. $\dot{M}_j^{(i)}$ is the mass flow rate of stream j which may be an input or an output stream, x_{kj} is the mass fraction of chemical k in stream j, and ψ_{k} is the specific potential environmental impact of chemical k. $\dot{I}_{\text{we}}^{(\text{cp})}$ is the rate of potential environmental impact output due to the emission from the chemical process. $\dot{E}_j^{(\text{cp})}$ is the rate of waste energy emission from the chemical process and ψ_{we} **is the potential environmental impact for energy emission which is assumed to be zero** [6].

The expressions for the energy generation process are analogous to the expression for the chemical process.

$$\dot{I}_{\text{in}}^{(\text{ep})} = \sum_{j}^{\text{ep}} \dot{I}_j^{(\text{in})} = \sum_{j}^{\text{ep}} \dot{M}_j^{(\text{in})} \sum_{k} x_{kj}\, \psi_k + \ldots \approx 0$$

$$\dot{I}_{\text{out}}^{(\text{ep})} = \sum_{j}^{\text{ep}} I_j^{(\text{out})} = \sum_{j}^{\text{ep-g}} \dot{M}_j^{(\text{out})} \sum_{k} x_{kj}\, \psi_k + \tag{A5}$$

$$\sum_{j}^{\text{ep-s}} \dot{M}_j^{(\text{out})} \sum_{k} x_{kj} \psi_k +$$

$$\ldots \approx \sum_{j}^{\text{ep-g}} \dot{M}_j^{(\text{out})} \sum_{k} x_{kj} \psi_k + \ldots \tag{A6}$$

$$\dot{I}_{\text{we}}^{(\text{ep})} = \sum_{j}^{\text{ep}} \dot{E}_j^{(\text{ep})} \psi_{\text{we}} \approx 0 \tag{A7}$$

where $\dot{I}_i^{(\text{ep})}$ is the rate of potential environmental impact in (i = in) or out (i = out) of the energy generation process; $\dot{I}_{\text{we}}^{(\text{ep})}$ is the rate of potential environmental impact output due to the emission of waste energy from the energy generation process; $\dot{E}_j^{(\text{ep})}$ is the rate of waste energy emission from the energy generation process; and ψ_{we} is the potential environmental impact for the waste energy emission. For the input, $\dot{I}_i^{(\text{ep})}$ and the waste energy, $\dot{I}_{\text{we}}^{(\text{ep})}$ the sums over j and k are respectively taken over all input or all output streams and all components k associated with the energy generation process. For the output, $\dot{I}_{\text{out}}^{(\text{ep})}$, the sum over streams j is broken into a sum over gaseous output streams, ep-g, and another sum over solid output streams, ep-s. The potential environmental impact of the solid output streams can be assumed to be negligible compared to that of the gaseous output streams [6].

The potential environmental impact of the mass inputs, $\dot{I}_{\text{in}}^{(\text{ep})}$, to the energy generation process is also assumed to be approximately zero. The energy generation process is assumed to be a coal-fired electrical power plant. The ψ_k for the components in coal is approximately set to zero. The air and the water have no potential environmental impact so ψ_{air} and ψ_{water} are set to zero and $\dot{I}_{\text{air}}^{(\text{in})}$ and $\dot{I}_{\text{water}}^{(\text{in})}$, are, consequently, zero. Summarizing, all of the terms under the summation can be approximately set to zero so that the entire term $\dot{I}_{\text{in}}^{(\text{ep})}$ is zero or at least very small compared to the output term, $\dot{I}_{\text{out}}^{(\text{ep})}$ [6].

The potential environmental impact of the mass outputs, $\dot{I}_{\text{out}}^{(\text{ep})}$, from the energy generation process are divided into gaseous and solid streams, as already mentioned. The gaseous streams mainly consist of air pollutants, e.g. NO_x, CO_2, SO_2, etc., and they are included in the analysis. The solid streams consist of coal slag, i.e. noncombustible ashes and residue, and coal impurities. It is assumed here that the potential environmental impact of the components in the solid output streams is negligibly small [6].

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