Evaluating Waste Minimization Alternatives in a Chemical Plant

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Abstract

Growing environmental concerns have spurred technological challenges within the chemical process industries to accommodate the concept of waste minimization. Commercial process simulators such as Aspen Plus, HYSYS, Pro II and ChemCAD, which have been extensively employed to solve plant synthesis problems, are also gaining currencies for achieving the desired waste minimization objectives. However, the use of these simulators is not a straightforward task as it requires considerable know-how, skills and expertise of the user for recognizing the process variables, which hold keys to the overall waste feature of the plant. In this paper, we present an integrated framework comprising of G2 expert system and HYSYS simulator to automate the overall waste minimization procedure. The framework has been developed by extending our previous ENVOP*Expert* system. Our updated ENVOP*Expert* capitalizes on the CAPE-OPEN capability of HYSYS process simulator through XML data technology. We illustrate the automated approach using an industrial hydrocarbon separation process from literature.

1. Introduction

Design of a chemical process involves a combination of synthesis, analysis and evaluation of different design alternatives. Such activities have been traditionally driven by economic factors first, followed by engineering, safety and environmental as the last priority. The result is often excessive add-on safety features and end-of-pipe treatment to reduce the consequences of acute hazards and environmental effects of a release. Increased cost competition, demand for consistently high product quality and stricter safety and environmental regulations have forced process designers to accommodate inherent safety and waste minimization principles starting from the early stage of process design. Process simulators have been proven useful in this regard as they allow comparison between the different design alternatives at shorter time without the need for extensive experimentation.

Literature has been abundant with articles on the applications of commercial process simulators to support the development of processes that are environmentally friendly and cost effective. Cabezas *et al* (1999) implemented a methodology called Waste Reduction (WAR) algorithm into CHEMCAD simulator to evaluate the environmental impact due

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to process modifications. Dantus and High (1999) combined compromise programming method with stochastic annealing algorithm using ASPEN PLUS simulator to simultaneously maximize the profit and minimize the environmental impact of a given chemical process. Chen and Shonnard (2003) utilized HYSYS simulator as a screening tool to assess the economic and environmental performances of a process. While these simulators are useful for solving the design problems, their use is still not a straightforward task as it requires considerable know-how, skills and expertise of the user for recognizing the process variables that hold keys to the overall waste feature of the process plant. And for such task, very little help is actually provided by these simulators.

Previously, we have reported on our attempt to automate the waste minimization procedure through integration between an expert system with HYSYS simulator (Halim and Srinivasan, 2002a). We have developed a system, called ENVOP*Expert* to automatically identify the sources of waste in a chemical process, propose process design changes to minimize them and simultaneously calculate the environmental impact and plant profitability. However to achieve the mentioned tasks, the user is required to switch over from G2 to HYSYS platform and vice versa during the procedure. In this paper, we present an improved ENVOP*Expert* by capitalizing on the CAPE-OPEN functionality of the HYSYS simulator. In our new framework, ENVOP*Expert* will operate as a decision support tool by accessing the physical property, process chemistry and flowsheet information of the HYSYS simulator through XML data transfer. Once such information is retrieved, ENVOP*Expert* will perform a two-step waste minimization assessment: waste source detection and waste minimization alternative generation.

2. Integrated Framework of ENVOP*Expert* and HYSYS

The CAPE-OPEN project, which started in early 1997, has enabled process simulation software to interoperate to support the process modeling and simulation needs (Braunschweig *et al*, 2000). Examples of such interoperation include property sharing between HYSYS and ASPEN PLUS, simulation interface between FLUENT and ASPEN PLUS, and OLE (Object Linking and Embedding) automation between HYSYS and Excel. Another useful tool that has been identified for collaborative CAPE environments is XML technology, a text-based markup language for representing and sharing data on the web. As HYSYS simulator has included XML and OLE HYSYS-Excel capabilities in its simulation engine, we have thus implemented these two features as integral parts of the ENVOP*Expert* system.

ENVOP*Expert* has been implemented in an object-oriented framework with the following task: *Given information concerning the process in the form of flowsheet, process chemistry and material information, it can automatically detect the waste components in the process, diagnose the sources where they originate and suggest intelligent design alternatives to eliminate or minimize them*. Figure 1 shows the overall framework of ENVOP*Expert*. First, a base-case process flowsheet that is developed in HYSYS is stored as an XML file. The XML data, which consists of flowsheet configuration, process chemistry and user's defined variables, is then passed as an input to the ENVOP*Expert* system. This information is then augmented using a P-graph model, which is a directed bipartite graph for representing a process structure (Friedler *et al*, 1994). In the P-graph model, a circle is used to represent a material stream, while a bar is an operating unit. A directed arc connects a material stream with an operating unit. This P-graph representation of a process provides a convenient framework for diagnosing the origins of waste in the process and for deriving qualitative waste minimization solutions. The reader is referred to Halim and Srinivasan (2002 b, c) for detailed discussion of the P-graph based analysis and waste minimization heuristics.

Once the qualitative solutions have been proposed, they can be detailed further using quantitative simulation. For this purpose, we have developed an ActiveX connection program in the G2 system and linked it with an Excel-VBA (Visual Basic for Applications) of AspenTech. Besides the simulation methods and procedures, the Excel program also contains process information data such as chemical environmental impacts and plant unit costs. In this way, any changes in the process variables proposed by ENVOP*Expert* will be passed to HYSYS for simulation with the results obtained transferred from HYSYS back to ENVOP*Expert* and analyzed for their environmental impacts and plant costs. Any synergies and trade-offs between different waste minimization alternatives will also be highlighted through plotting of these two factors.

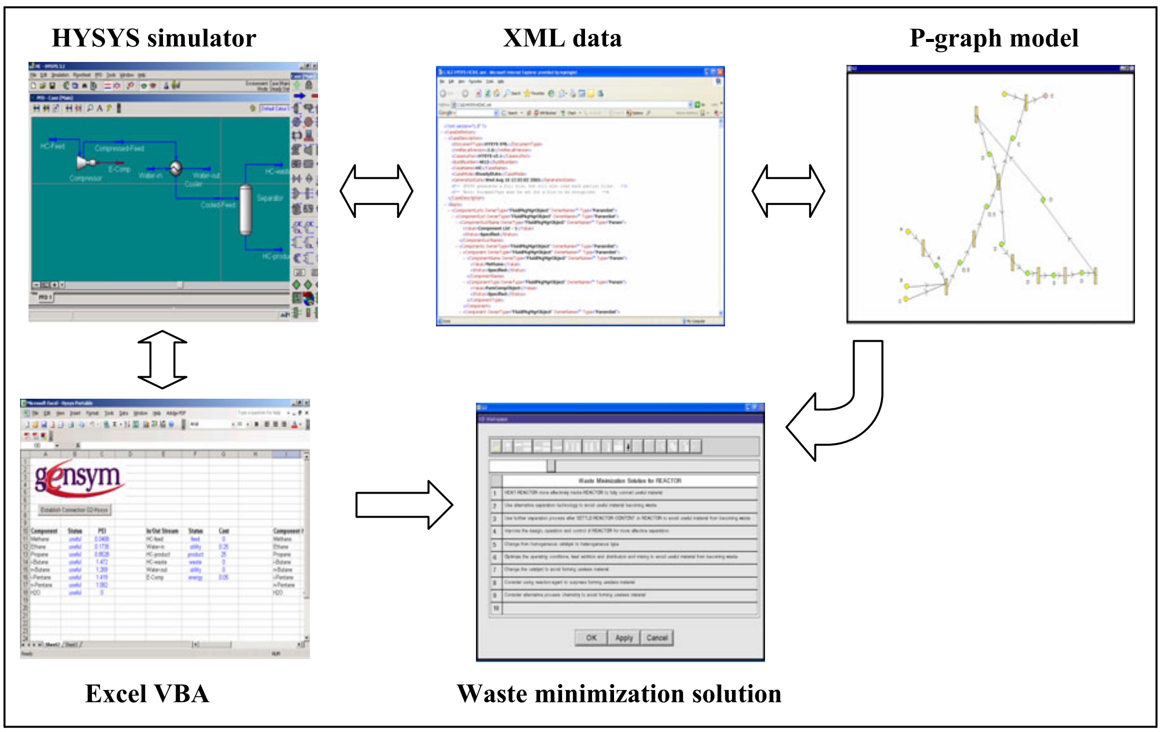

Figure 1. ENVOPExpert Framework

3. Case Study: Hydrocarbon Separation Process

We illustrate our automated approach using an industrial hydrocarbon separation case study (Isalski, 1995). Figure 2 shows the basic flowsheet of the process. An incoming vapor stream containing a mixture of hydrocarbons (C1 to C5) is initially compressed to a high pressure in the feed-compressor followed by condensation using cooling water in a heat exchanger. The resulting vapor-liquid mixture is flashed in a separator from which the liquid from the bottom is used as product. The vapor from the top is a waste and is sent to a flare system. Table 1 shows the unit costs and the WAR based environmental impacts of the material components of the process.

Table 1. Unit cost basis and environmental impact factors

Component	Environmental impact (mol basis)	Stream	Cost
Methane	0.0026	Dried HC-vapor	0
Ethane	0.0058	Cooling-water in	$0.0045/kmol
Propane	0.0194	Oil export	$5/kmol
i-Butane	0.0254	Flared HC	0
n-Butane	0.0219	Cooling-water out	0
i-Pentane	0.0197	C3-energy	$0.05/kWh
n-Pentane	0.015		

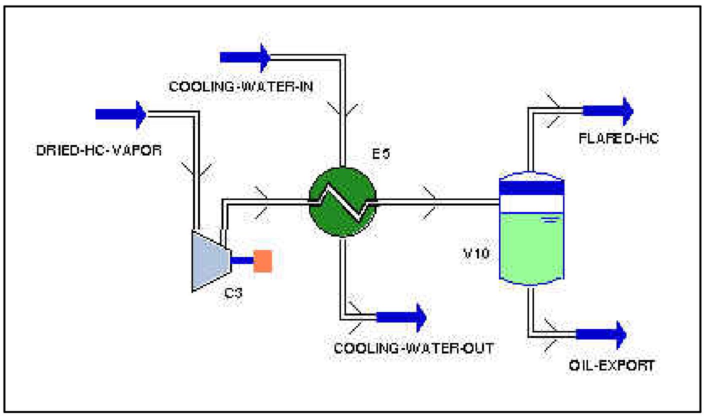

Figure 2. Flowsheet of hydrocarbon separation process

A qualitative review has been carried out for this process with the objective of reducing the hydrocarbon vapor sent to the flare system. Table 2 summarizes the qualitative solutions of ENVOP*Expert*. The reader is referred to Halim and Srinivasan (2002b) for detailed procedure for deriving those solutions.

Next, quantitative analysis is performed for analyzing the environmental impact and the plant cost. Table 3 shows the tabulated results caused by five percent changes in various process variables. As shown in the table, both the environmental impact and the process operating cost can be reduced through 5% increase of the feed pressure and 5% decrease of the feed temperature and the cooling water temperature. On the other hand, an alternative of “decreasing the component flowrate in the feed stream”, which reduces the environmental impacts, does not necessarily reduce the operating costs. This signifies a trade-off between the operating cost and the environmental impact for such alternative. Optimal operating condition that simultaneously minimizes the environmental impact and the process cost can also be found. The results in the table show that “decreasing the flowrate of methane" would yield a significant improvement to both the environmental impact and the plant operating cost.

Table 2. Qualitative waste minimization solutions of ENVOPExpert

Source	Waste minimization solution
Feed stream	Prevent excessive hydrocarbon feed Decrease temperature of hydrocarbon feed
Compressor	Increase compressor energy Improve compressor design
Heat exchanger	Increase flow rate of cooling water Decrease temperature of cooling water Improve heat exchanger design Use alternative cooling agent
Separator	Improve separator design
Waste stream	Recycling of vapor waste stream

Table 3. Waste minimization simulation of ENVOPExpert

Source	Waste minimization solution	Environmental impact	Plant operating cost ($)
	Base case	53.5	-424
Feed stream	Decrease temperature	53.4	-388
	Increase pressure	53.1	-304
	Decrease molar flow of methane	51.7	-84
	Decrease molar flow of ethane	53.0	-388
	Decrease molar flow of propane	52.6	-484
	Decrease molar flow of i-butane	53.3	-483
	Decrease molar flow of n-butane	53.5	-435
	Increase molar flow of i-pentane	53.5	-349
	Increase molar flow of n-pentane	53.5	-420
Compressor	Increase power	53.5	-424
Cooling water stream	Decrease temperature	53.3	-358
	Increase flowrate of water	53.5	-459

4. Conclusions

The issue of waste minimization has challenged the chemical industries to initiate new approaches to tackle waste problems. We have developed a methodology for automating identification of waste minimization strategies in the chemical processes and successfully implemented it as an intelligent system called ENVOP*Expert*. ENVOP*Expert* has been developed by integrating an expert system with a commercial process simulator and shown capable in generating waste minimization solutions both in qualitative and quantitative manner. We have successfully tested our system on a hydrocarbon process and planned to include automatic optimization procedure into the current framework in future.

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