Development of a Pollution Prevention Tool for Design of Continuous Chemical Processes

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Abstract

Performing a pollution prevention assessment of a chemical process design is typically resource intensive. Time constraints, a lack of resources and limited in-house expertise, particularly in developing nations, have resulted in inconsistent and non-routine identification of pollution prevention opportunities. To address these problems, computer based tools may be developed to enable designers to rapidly understand environmental implications and provide suggestions of process modifications. A software prototype, P2TCP (Pollution Prevention Tool for Continuous Processes) is presented. P2TCP provides support and helps facilitate pollution prevention assessments of continuous chemical processes at all stages of design.

There is a significant need for quantitative methods for comparison of process alternatives. Although chemical and safety hazard rating schemes have a long history, there is no universally accepted method for comparison in terms of potential environmental impacts. Full health and environmental risk analysis is not suitable for conceptual process design decision making but models or indicators can provide a suitable approach. A number of methods are incorporated in P2TCP.

The benefits of heat and mass integration tools for pollution prevention (P2) have been widely demonstrated. However no tool has been developed specifically to assist in the intuitive process of systematically identifying alternatives for continuous chemical processes which may reduce waste generation and energy consumption. P2TCP incorporates an expert system for P2 design analysis which is complementary to existing integration and simulation tools. The key features of the analysis system are presented.

Keywords

Chemical process design analysis, environmental comparison, pollution prevention

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1 INTRODUCTION

The chemical process industries face continually increasing pressure from society and legislation to reduce releases to the environment. Over the past 20 years, waste treatment methods have provided sufficient control against environmental impact for compliance with media specific legislation. As legislation strengthens and impact to all media is simultaneously considered, treatment processes alone no longer provide a cost effective solution. Good house keeping and elimination of some fugitive emissions have demonstrated impressive reduction results with good returns. However, further reductions of wastes and reliance on treatment may be achieved through modification of designs. The identification of modifications and comparison of alternatives is termed a pollution prevention (P2) assessment.

Performing a P2 assessment is typically resource intensive and particularly not suitable to provide decision making during conceptual process design. An informal survey (Fromm 1992) of several process design and project engineers indicated that "P2 is practised in design but not consistently, routinely or in the form of specific design criteria" but typically as a result of reducing material loss, toxic release and avoidance of costly treatment, reflected by an engineer's personal awareness and experience. To address these problems, computer based tools may be developed which enable designers to rapidly understand environmental implications and to suggest alternatives.

Process design simulation tools facilitate the creation of process flow diagrams and provide estimates of waste quantities. However the use of these tools for pollution prevention assessment are limited because they do not incorporate systems for environmental comparison or identification of potential modifications.

Development of an appropriate environmental methodology to date is limited. (Brennan 1992, SERC 1993). Available methods to identify design alternatives still require expert knowledge, a significant number of "skilled" man hours and applicability of these methods, particularly during conceptual process design, is limited. (Fromm 1992, Hethcoat 1990)

P2TCP (Pollution Prevention Tool for Continuous Processes) is a computer based prototype which was developed to assist in the comparison of process alternatives and the identification of potential modifications to reduce environmental impacts. P2TCP is presented in this paper.

2 OVERVIEW OF P2TCP

The prototype of P2TCP includes four modules for P2 design analysis and the generation of environmental comparison data. The structure of P2TCP is presented in figure 1.

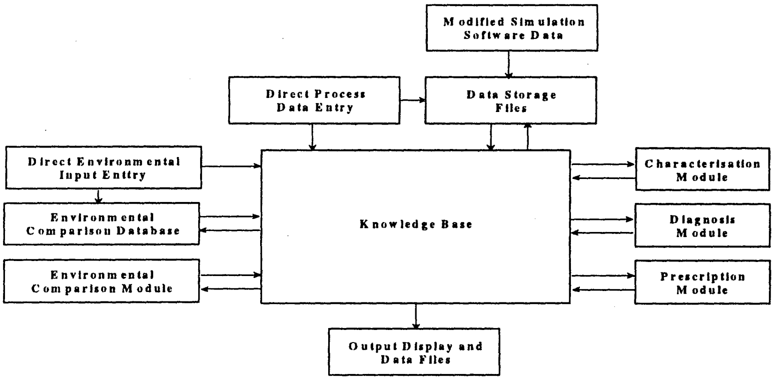

Figure 1 Structure of P2TCP.

Process design information may be input manually or retrieved from data files. Data files may be partially generated from modified process simulation files. Design information of a chemical process is represented in the knowledge base. The knowledge base provides storage for design data and assessment results. Results can be previewed on screen and exported to data files.

Process waste streams may be compared on an environmental basis. A number of environmental comparison methodologies are represented in P2TCP, see section 4. Property data required for each methodology may be retrieved from a database or directly input through a user interface.

The consecutive processes involved in the analysis of a design are represented by three modules, see section 5. Process design data are classified in the characterisation module. Then interactions of a process are determined in the diagnosis module. Once components have been classified and interactions diagnosed, analysis is performed using the prescription module.

3 SOFTWARE REPRESENTATION

P2TCP is represented in KAPPA PC (Intellicorp). KAPPA PC is a knowledge-based systems shell. The shell incorporates an extensive range of processing tools, interface capabilities and is suitable for different prototype development stages. Support is available through an on-line news group.

Process design information and assessment results are represented in the knowledge base as objects. Objects are either classes or instances, in a hierarchical structure. Characterisation, diagnosis and environmental comparison modules are based on functions, general procedures. Heuristics are represented as rules in the prescription module. All rule premises are defined by either user inputs or diagnosis and therefore prescription rules do not involve chaining. Rules and functions are not specific to particular objects.

4 ENVIRONMENTAL COMPARISON MODULE

A significant need has been identified for methodologies, based on scientific principles, for comparison of processes during different stages of design. (Brennan 1992, SERC 1993) Consideration of environmental impacts during conceptual and retrofit design has a significant number of advantages which include:

- increasing decision makers' awareness of environmental considerations
- selection and justification of process alternatives
- establishing source reduction goals and measuring progress.
- reduction of potential risks and future liabilities
- compliance with management standards and objectives.

A number of methodologies have been presented in literature to prioritise and measure reduction efforts. (Pennington) To aid in selection, methods can be considered in the context of a hierarchy based on effect and exposure considerations, Table 1. However this hierarchy is not a rigid classification.

Table 1 Hierarchy of Quantitative Regional Comparison Techniques (Pennington)

Complexity	*Technique*	*Effect*	*Exposure*
low	direct data summation	none	none
↓	effect normalisation	legislative criteria	none or incorporated in criteria
↓	score and ranking	selected criteria	selected criteria
↓	exposure concentration modelling	selected criteria	model predictions
high	full impact assessment	all significant effects	all exposure pathways and criteria

Available methodologies may be limited by their ability to represent the relative environmental behaviour of effluent components, intrinsic uncertainty, and variation in data. These limitations are not typically quantified.

Comparison techniques in P2TCP are based on potential long term, low concentration exposure effects associated with continuous chemical releases, i.e. regional and global scale effects. To reflect potential impacts which are considered to be of relatively high or medium risk (US EPA 1990), the following methodologies are incorporated:

- waste distribution analysis based on process inventory data
- a multi-compartment model, using readily available data, associated assumptions and an estimation of uncertainty, for regional comparison in terms of Relative Impact Potentials (RIPs) (Pennington 1997)
- a number of global impact comparison potentials

Uncertainties associated with RIPs are quantified.

5 P2 DESIGN ANALYSIS MODULES

Expert systems provide a basis for the representation of knowledge in the form of heuristics. Expert systems may be used to reduce limitations associated with P2 knowledge and resources leading to improved process design through the generation of alternatives. P2TCP incorporates an expert system to provide an analysis of process designs. The analysis results provide a basis to identify alternatives which may reduce intrinsic waste generation and energy consumption. This system is complementary to existing integration and simulation tools.

P2 design analysis may just relate to a single process unit operation. This operation may then be modified to provide environmental improvements. However other unit operations may be adversely affected and result in greater environmental impacts (material discharge or energy consumption). P2TCP incorporates an analysis system for continuous chemical processes which considers both individual unit operations and their interactions.

To determine the cause of a fault and subsequent solutions it is necessary to know what the fault is and identify potential interacting variables. In P2TCP process waste streams, components and reactions are classified using functions to provide a basis for subsequent diagnosis and prescription.

Once a fault has been identified it is necessary to determine the potential interactions within a system which may effect this fault and affect others. In

P2TCP the potential interactions within a process are identified in the diagnosis module.

Knowing a fault and the potential interactions within a system it is necessary to identify how the system may be manipulated to limit the fault. In P2TCP, analysis is performed using heuristics to help identify potential opportunities and conflicts which may result in reduced waste generation and energy consumption.

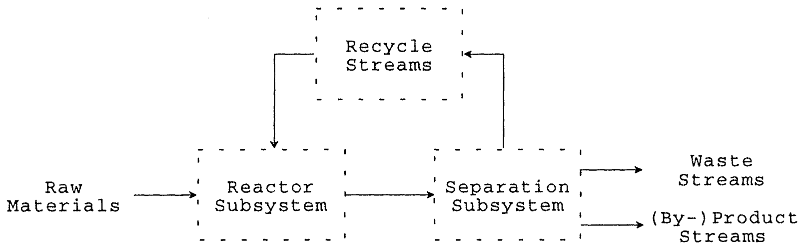

Figure 2 Subsystems and their Interactions Represented in P2TCP

Heuristics were systematically developed for P2TCP from generic design principles to provide detailed analysis which does not require the specification of a base case. A classification system related to the generic structure of processes, see figure 2, was used to avoid representation of P2 heuristics on an ad-hoc basis and facilitate the incorporation of pollution prevention assessments into conceptual design at increasing levels of complexity.

6 CASE STUDIES

Case studies using P2TCP demonstrated that the RIP model may provide a discriminatory basis for the comparison of process effluents for a given 'idealised' situation, i.e. for specific compartment volume ratios. (Pennington 1997) However, estimates of uncertainty indicate that while such multi-compartment models provide an indication of compartments which may be affected, they are not applicable for fine distinction amongst effluents which exhibit similar behaviour unless accurate input data are available.

The affects of operating conditions, reactor type and thermal mode on the reaction system of the allyl chloride chlorination process were determined using a simulation package and P2TCP. Affects on selectivity, raw material conversion, energy generation and energy distribution were considered. The predictions of P2TCP corresponded with the results from the simulation models and presented in literature. The time required to identify interactions and potential modifications was significantly less using P2TCP. However the relative significance of affects was not determined.

Separation alternatives and generic advice related to process interactions for the allyl chloride production process were determined. The alternatives identified included the typical industrial techniques. Based on the program output, the range of feasibility of the different alternatives was considered. The generic advice related to potential interactions in the process was used in combination with the feasibility ranges of the separation alternatives to identify a number of options which may reduce the generation of waste and energy consumption.

7 CONCLUSION

A prototype of P2TCP (Pollution Prevention Tool for Continuous Processes) has been developed in response to the demand for a computer based pollution prevention assessment systems which compliments existing mass and heat integration tools. P2TCP comprises of modules for environmental comparison and P2 design analysis of continuous chemical processes. P2TCP is suitable for structured conceptual and retrofit design. The prototype has been validated using a number of case studies.

A number of environmental methodologies have been presented in literature which may be used for computer based comparison of process alternatives. However, no single methodology is appropriate for all situations and uncertainty is typically un-quantified. Several regional and global comparison methodologies which reflect the current state-of-the-art are incorporated into the environmental comparison module of P2TCP.

In P2TCP, three modules represent the consecutive processes required for P2 design analysis; characterisation, diagnosis and prescription. Three process sub-systems are considered which correspond to levels 2 to 4 of hierarchical design. Conflicts within and between sub-systems are identified, including between energy consumption and waste reduction.

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10 BIOGRAPHY

David William Pennington is a Research Assistant in the Department of Chemical Engineering at the Hong Kong University of Science and Technology (HKUST). In 1990, having successfully completed one year of industrial training, he graduated from Surrey University in England with a B.Eng. in Chemical and Process Engineering. Prior to joining the Ph.D. program at HKUST in 1993, he worked as a consultant with Advanced Mechanics & Engineering Ltd. in England. A thesis related to the development of the software described in this paper, P2TCP, will be submitted in early 1997 as partial fulfilment of the requirements for a Ph.D. in Chemical Engineering.