INTEGRATED APPROACH FOR POLLUTION PREVENTION IN PROCESS DESIGN AND DECISION-MAKING

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by

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Abstract

Pollution prevention (P2) has gained significant importance over pollution control strategies to manage environmental issues in process industries. P2 reduces the hazardous emissions via mass and energy conservation and thus leads towards sustainable development.

The present work has developed a holistic P2 approach to facilitate the successful implementation of the P2 program in process industries. The greater P2 opportunities exist in the preliminary design phase; therefore, to contribute in this area the present research has developed a structured process design approach, SusDesign. It integrates numerous tools, such as exergy and energy analysis, process integration, cogeneration, trigeneration, etc., with a process simulator, Aspen HYSYS. This integration assists the designers to systematically generate and analyze design alternatives at different design stages.

A detailed algorithm has also been developed to carry out structural and parametric optimizations of a process flowsheet. The most important feature of the SusDesign approach is that it uses quantitative techniques to evaluate the environmental and cost performance of design options by imbedding the IECP approach, developed as a part of this work. The IECP tool is integrated with the Aspen HYSYS for quantitative evaluation, screening and optimization of the investigated design options.

The application of the SusDesign approach has been demonstrated through the design of a 30 MW thermal power plant. Compared to the conventional gas turbine

power plant, the final design has achieved an improvement of overall thermal efficiency of the plant by about 35% and the reduction of CO_2 and NO emissions by about 49% and 80% respectively.

The applicability of the IECP approach has been demonstrated through a separate case study, where potential NOx reduction options are evaluated in a 125 MW thermal power plant.

In the final phase of this research, a risk-based environmental assessment approach, E-Green, has been developed for the detailed environmental evaluation of a flowsheet. E-Green has been implemented in combination with the Aspen HYSYS to assess two different solvent options in an acrylic acid manufacturing plant.

Acknowledgement

All praises are for Al-Mighty Allah, who has given me the opportunity to complete this work despite having so many problems.

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List of Abbreviations

CP	Cost potential
FGR	Flue gas recirculation
HRSG	Heat recovery steam generator
IECP	Integrated environment and cost potential
LCA	Life cycle assessment
NO	Nitric oxide
NOx	Oxides of Nitrogen
P2	Pollution prevention
P2P	Pollution prevention potential
SI	Steam injection
TWS	Total weighted score
UOFC	Unit operating and fixed cost
WI	Water injection

List of Symbols

E	Total exergy of a system
E^{CH}	Chemical exergy
e_f	Flow exergy
E^{kN}	Kinetic exergy
E^{PH}	Physical exergy
E^{PT}	Potential exergy
$\bar{e}_F^{ch}$	Specific chemical exergy of a fuel
$\dot{E}_d$	Exergy Destruction rate
$\dot{e}_d$	Exergy destruction rate for unit mass
$\bar{g}$	Gibbs function
g	Gravitational acceleration
h	Specific enthalpy at a given state
h_o	Specific enthalpy at reference environment temperature
$\bar{h}$	Heat of formation
$R_{\text{in Cat-k}}$	Risk due to the handling of all input materials to an impact category *k*
$R_{\text{LCA raw cat-k}}$	Risk to an impact category *k* due to the emissions over cradle-to-gate life cycle domain (i.e. raw materials production and supply domain)
$R_{\text{out Cat-k}}$	Risk to an impact category *k* due to all product and waste streams
$R_{\text{pros cat-k}}$	Risk to an impact category *k* due to the emissions over process gate-to-gate domain
$R_{\text{pros energy cat-k}}$	Risk to an impact category *k* due to the emissions concerned with the production of energy consumed in a process unit
$R_{\text{tot cat-k}}$	Total risk to an impact category *k*

$R_{m\ Cat\text{-}k}$	Risk to an impact category *k* due to the emissions related to the production and supply of a raw material *m*
S	Entropy at given state
S_o	Entropy at reference environment
$\bar{s}$	Absolute entropy
To	Temperature of the reference environment
T_o	Temperature of the reference environment
U	Internal energy
U_o	Internal energy at reference temperature
V	Velocity at a given state
V_o	Velocity at reference temperature
y^e	Mole fraction of any component at reference environment
y^i	Mole fraction of any given component
$\dot{W}_{cv}$	Work output rate in a control volume
z	Elevation

Greek Symbols

$\psi_{c,j,s,k}$	Risk to an impact category *k* due to a component *c* of a waste stream *j* in a production step *s*
$\psi_{e,k,s}$	Risk to an impact category *k* due to the emissions associated with the production of the energy consumed in a production step *s*
$\psi_{t,k,q}$	Risk to an impact category *k* due to the emissions from a transportation step *q*
$\psi_{i,k}$	Risk for handling of an input material stream *i* to an impact category *k*
$\psi_{p,\ k}$	Risk to an impact category *k* due to a product stream *p*
$\psi_{c,j,\ k}$	Risk to an impact category *k* due to the release of a component *c* in a waste stream *j*

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Chapter 1

Introduction and Overview

1.0 Introduction

Concern over global climate change is pressing manufacturers to employ better environmental management strategies for controlling pollutants discharged to the environment. The traditional end-of-pipe pollution control approach to environmental management does not produce robust and cost effective solutions for continuous improvement of environmental quality. Therefore, a shift towards pollution prevention (P2) strategies has been promoted by governments, industries, and individuals for sustainable environmental management.

With the Pollution Prevention Act, the U.S. Congress established pollution prevention as a "national objective" and the most important component of the environmental management hierarchy (US EPA, 1990). Through the approval of the Canadian Environmental Protection Act, the government of Canada is also committed to implementing pollution prevention as a national goal and as the priority approach to environmental protection to achieve sustainable development (CEPA, 1999). Many other regulatory regimes have also recognized P2 as a powerful tool to minimize pollutants generation and reduce the potential threats to human health and eco-systems (Environment Canada, 1994).

P2 provides significant advantages over end-of-pipe pollution control, which include reduced production cost, risk, and resulting liability, improved competitiveness, and enhanced customer trust. In this way, P2 can play an important role towards the development of green and economically viable process. For successful implementation of P2 during preliminary process designs and retrofit activities, a detailed and systematic P2 approach is required. Though there are a few approaches in practice, still there is no holistic P2 approach to assist the designers for the systematic development of sustainable process systems. Following are the major limitations that were observed in most of the published approaches (Section 2.1.4, chapter 3):

- Lack of the consideration of global system boundary during the generation of P2 alternatives; therefore, in present process systems, P2 alternatives consider only pollution mitigation from the plant boundary. This cannot alleviate the global emission problem.
- Lack of consideration of other environmental management options along with the P2 options during the final decision making.
- Lack of consideration of risk and safety criteria as an objective function during the feasibility analysis of different P2 options.

In practice, in the implementation of a P2 approach, designers encounter the following challenges:

- Method to generate different design options employing different P2 strategies in a systematic manner during the preliminary process design or retrofit applications.

- Methods/tools to evaluate the generated P2 options in terms of environmental, technical and risk and safety criteria.

These challenges are due to the lack of adequate approaches or tools, therefore, the objectives of the present work are to resolve the above issues by:

- Developing an integrated pollution prevention methodology (IP2M) for systematic implementation of P2 program in process industries.
- Developing a process design approach which facilitates the generation of different alternative design options by employing P2 strategies at different stages of a preliminary process design and retrofit activity.
- Developing a robust risk-based environmental assessment approach to support the environmental evaluation of the P2 options.

1.1 Overview of the Thesis

This thesis is written in manuscript format. It combines a number of manuscripts either published or submitted to journals for possible publication. The organization of the thesis follows the guidelines approved by the Faculty of Engineering and Applied Science of Memorial University of Newfoundland.

Chapter two provides a detailed literature review to give support to the reader for understanding different manuscripts. In order to avoid unnecessary duplication, the literature review does not include the topics which have already been discussed in more detail in different manuscripts chapters.

Chapter three is a manuscript, which reviews different existing P2 approaches and finally proposes an integrated pollution prevention approach (IP2M) for practicing in process industries. This manuscript has been published in the journal of Hazardous Materials.

A process design approach (Susdesign) is developed by employing different P2 strategies in concert with a number of engineering tools has been developed. The different elements of the SusDesign approach along with its application in designing a 30 MW thermal power plant has been described in manuscript chapter four. This manuscript has been submitted to the Applied Thermal Engineering journal for possible publication.

In the proposed process design approach (SusDesign), the alternative design options generated at the preliminary process design are evaluated based on environmental and economic performance. At this point, for quick evaluation, an integrated environmental and cost and potential (IECP) index has been developed by employing the proposed IECP approach. The details of the IECP approach and its application to evaluate different alternatives for NOx reduction in a 120 MW thermal power plant has been described in manuscript chapter five. This manuscript has been submitted for possible publication to the journal of Energy for Sustainable Development.

One of the major steps of the IP2M approach is the detailed environmental evaluation of different complete P2 options or candidate flowsheets. For this, a robust risk based environmental evaluation approach (E-Green) has been developed and described in manuscript chapter six. This manuscript has already been published in the journal of Industrial Engineering and Chemistry Research.

Finally, chapter seven describes the conclusions, novelties and recommendations for the future work necessary to be carried out in this particular area of research.

Chapter 2

Literature Review

The objective of this chapter is to provide a detailed literature review to give support to the readers to understand different manuscript chapters. Therefore, it only includes the topics which are discussed briefly in the manuscripts. This chapter provides basic information about pollution prevention (P2), different P2 opportunity assessment tools and environmental impact assessment methods. Furthermore, it also provides a literature review on exergy analysis and its application to the performance improvement of different thermal power plants.

2.0 Definition of Pollution Prevention

Pollution prevention is defined by Environment Canada National Office of Pollution Prevention as "The use of processes, practices, materials or energy that avoid or minimize the creation of pollutants and wastes without creating or shifting new risks to communities, workers, consumers or the environment,"(Wolnik and Fischer, 2005). While in the US Pollution Prevention act 1990, pollution is defined as "any practice which reduces the amount of a hazardous substance, pollutant, or contaminant entering any waste stream or otherwise released into the environment (including fugitive emissions) prior to recycling, treatment, or disposal; and any practice which reduces the hazards to public health and the environment associated with the release of such substances, pollutants, or contaminants" (US EPA, 1990). From the above definitions it is apparent that P2 involves the judicious use of resources through source reduction, energy efficiency, reuse of input materials during production, and reduced water consumption. It is a multi-media approach, which includes the reduction of all sorts of releases such as air emissions, wastewater discharges, or solid waste involving the application of the best management practices, product changes, and modifications of manufacturing processes (US EPA, 1992).

Pollution prevention does not include any activities related to end-of-pipe control such as off-site recycling, waste treatment, concentrating and dilution of the toxic constituents, or transferring hazardous or toxic constituents from one medium to another.

2.1 Benefits of Pollution Prevention

Traditional end-of-pipe pollution abatement and control generally involves the use of complex technologies, requires large infrastructure and manpower, which increase compliance costs (Nourai et al, 2001, Hilson, 2000; Warren et al., 1999). In addition, in most cases it simply transfers pollutants from one medium to another. In contrast, pollution prevention can address the multi-media impacts of facilities or processes more effectively through source reduction measures.

Use of pollution prevention significantly reduces the waste load, which consequently reduces waste treatment and disposal costs and associated health concerns. Apart from that pollution prevention has some other benefits, including:

- reduced operating costs
- reduced materials costs
- reduced production costs
- improved business efficiency and profitability
- improved customer trust
- reduced regulatory compliance costs
- reduced future cleanup costs
- reduced future risk of liability
- reduced risk to workers and to the community

2.2 Environmental Management Hierarchy

US EPA has developed the Environmental Management Hierarchy and the Ontario Ministry of Environment and Energy has adopted this hierarchy model (Environment Canada, 1994). It provides the structured guidelines for environmental management. Highest priority is given to the pollution prevention through source reduction and in-process recycling. Other end-of-pipe treatment options such as off-site recycling, treatment and disposal have sequentially lower priority. According to the hierarchical approach, if the waste or pollution could not be completely removed even after employing the pollution prevention measures or none of the P2 measures are considered to be feasible, other non-pollution prevention measures should be implemented in hierarchy order.

2.3 P2 Opportunity Identification Tools

For the generation of design alternatives based on P2 strategies several thermodynamic tools are used. Some common are: exergy analysis, heat integration, mass integration, cogeneration /trigeneration etc. Apart from this life cycle assessment also could be served for the generation of P2 alternatives. The following sections briefly describe about these tools:

2.3.1 Heat Integration

Heat integration targets the minimum use of heat utility systems through the optimum use of the waste heat from process streams. It looks into all the hot or cold streams of the process system in order to achieve the following tasks:

i) Selection of which heating and cooling utilities could be used.
ii) The optimum amount of heating and cooling load that could be removed or added by each utility stream.

iii) Proper matching of the hot and cold streams.

iv) The configuration of the heat exchanger net works for optimal performance.

During each of the above task a number of pollution prevention opportunities would be obtained. Here, the pollution prevention target is achieved only through the reduction of the energy usage for heating and cooling operations. If electricity from grid is used for producing the hot utilities, then energy reduction via the use of heat integration does not make any significant difference in terms of pollution prevention if the local pollution is considered, therefore, in the proposed approach pollution over the wide system boundary has been considered through life cycle based impact assessment.

The heat integration is usually performed using pinch technology. Pinch point is a point that exists somewhere in the heat exchanging system, where the heat exchanging driving force is the minimum. For heat integration, three methods are generally used: i) temperature interval method, ii) graphical method and iii) linear programming (LP) method. Temperature interval method is the most common and easy to use without having any programming skill. This method is developed by Linnhoff and Flower (Linhoff and Flower, 1978). The method consists of the following four steps:

i) Choosing a minimum approach temperature in the heat exchangers, ΔT_{min}.

ii) Construction of a temperature-interval diagram.

iii) Development of total exchangeable heat load (TEHL) table.

iv) Construction of a cascade diagram.

Step 1. Choosing of a minimum approach temperature

Minimum approach temperature is the smallest temperature between a hot and a cold stream during the heat exchanging operation. Selection of minimum approach temperature has significant impact on energy load and heat exchanger size. While the minimum approach temperature increases, the heat transfer per unit area decreases, therefore the area of the heat exchanger decreases which leads to the smaller size heat exchanger. This results in less fixed capital cost. However, the energy load on the hot or cold utilities will be increased, which is not desired from pollution prevention perspective. Due to the increased use of the utilities the operating cost of the plant also will be increased. Therefore, a trade off is needed to optimally select the minimum.

Step 2. Construction of temperature interval diagram (TID)

This is a useful tool to insure the thermodynamic feasibility of the heat exchange between the hot and cold streams. In a temperature interval diagram all the hot streams and cold streams are represented vertically side by side. The hot streams that required to be cooled are drawn on the left side of the TID and cold streams that need to be heated up are shown on the right. According to the corresponding temperature scale all the hot streams and cold streams are represented therefore, the temperature axes of the hot and cold streams become shifted by the minimum approach temperature.

On the TID each stream is represented as a vertical arrow whose tail corresponds to the initial temperature of the stream, while its head represents the target temperature of the stream. Therefore, hot streams always drawn by top-to-down arrow and cold streams by down-to-top arrow. Horizontal lines are then drawn at the head and the tail of each arrow. These horizontal lines define the series of temperature intervals. The temperature intervals are numbered from top to bottom in an ascending order. The number of interval could be correlated with the number of total cold and hot streams by the following equation:

$$N_i \leq 2(N_h + N_c) - 1 \tag{2.1}$$

The equity only applies when no heads on any tails coincide. Within any interval heat transfer is feasible from the hot streams to the cold stream according to the second law of the thermodynamics. The driving force of this heat transfer is the existence of the minimum approach temperature difference between the hot and cold streams in each temperature interval.

Step 3. Development of total exchangeable heat load table

At this step, the exchangeable heat load is developed at each temperature interval for the process streams. For a hot stream *j*, the exchangeable heat load that passes through the *n*th interval is:

$$HEH_{j,n} = \dot{m}\, C_{p,j}\, (T_{n-1} - T_n) \tag{2.2}$$

Cp is the specific heat of the stream j and T_{n-1} and T_n are the hot scale temperatures at the top and the bottom boundary lines of the interval n. Similarly, the exchangeable capacity of the cold stream k which passes through the nth interval is computed from the following relation:

$$HEC_{k,n} = \dot{m}\, C_{p,k}\,(t_{n-1} - t_n) \qquad (2.3)$$

Where, $C_{p,k}$ is the specific heat of the kth cold stream and t_{n-1} and t_n are the cold scale temperatures for the upper and lower boundary lines of the interval n.

If more than one process streams are involved then total exchangeable loads for the hot and cold streams passing through a particular temperature interval n could be computed by using the following two equations:

$$HEH_n^{total} = \sum_{j=1}^{m} HEH_{j,n} \qquad (2.4)$$

$$HEC_n^{total} = \sum_{k=1}^{p} HEH_{k,n} \qquad (2.5)$$

Where, m and p are the number of hot streams and cold streams passing through the nth temperature interval.

Step 4. Construction of a cascade diagram

Cascade diagram represents the details heat balance around all temperature intervals. As discussed earlier that within each temperature interval, it is thermodynamically feasible to transfer heat from a hot stream to a cold stream. Besides, it is also possible to transfer the residual heat from a hot stream at a particular interval to a cold stream of the next lower interval due to the lower temperature of the cold stream. Therefore, for a particular temperature interval the energy balance equation can be written as follows:

$$HEH_n^{total} - HEC_n^{total} + H\,R_{n-1} - H\,R_n = 0 \qquad (2.6)$$

Where, HR_n is the residual heat load leaving the *n*th interval and HR_{n-1} is the residual heat load entering the *n*th interval. This is important to note that in order to be thermodynamically feasible the value of the residual heat loads must be positive. The negative values correspond that residual heat is flowing upward which is not feasible according to the second law of the thermodynamics, which states that heat can not be flowed from lower temperature to the higher temperature level without the aid of external work.

The first phase of a typical cascade diagram is shown in Figure 2.1. The figure shows that HR for the first interval is zero. This is due to the fact that no process stream exists above the first interval. The maximum non-negative residual exists at interval – which corresponds to the minimum heating utility requirement that needs to be added in order to make the heat exchanging systems thermodynamically feasible. Figure 2.2 shows the revised cascade diagram where this minimum heating utility requirement $Q^{min}_{heating}$ is added. In this figure the location at which the residual load becomes zero is called thermal pinch point. It is the same point where the maximum negative residual load exists in the initial cascade diagram. It indicates that no heat energy is transferred across the pinch point. The revised cascade diagram insures the requirements of the minimum amount of heating and cooling utilities. The residual heat that leaves from the last temperature interval corresponds to the minimum cooling utility requirement $Q^{min}_{cooling}$ to remove the heat in order to achieve the target temperature. The pinch point can also be located in terms of the corresponding hot scale and cold scale pinch point temperatures. Therefore, the heat integration based on the pinch technology uses the available process streams for the required heat exchange. It has twofold benefits; first, it saves the heat energy and thereby reduces the emissions to the environment and the second is that it

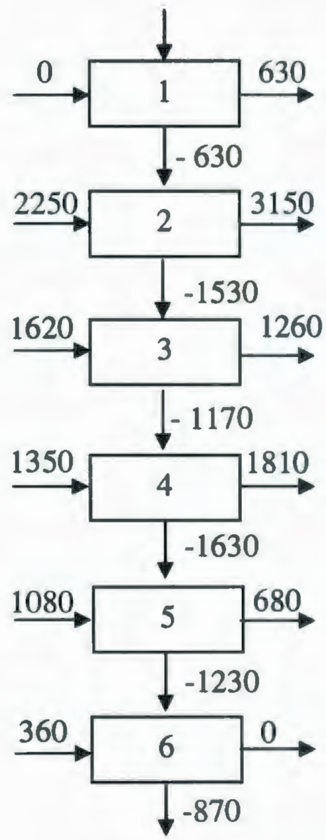

Figure 2.1: The Cascade Diagram

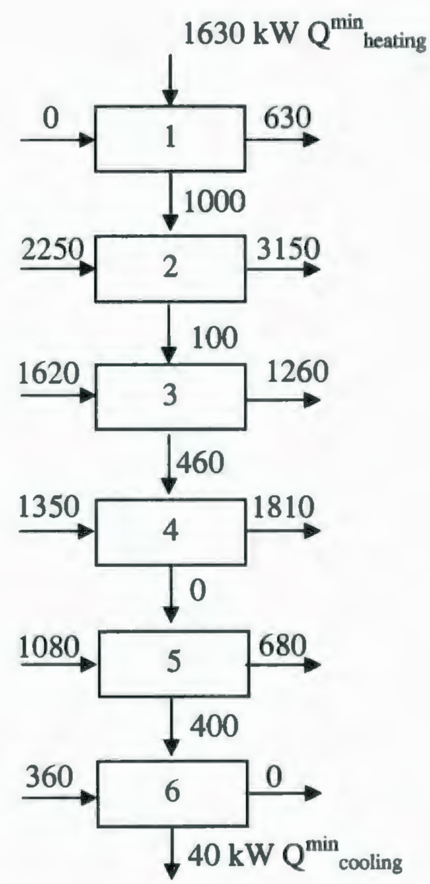

Figure 2.2: The Revised Cascade Diagram

insures the minimum operating cost for the heat exchange due to the use of minimum utility for heating or cooling.

2.3.2 Mass Integration

It deals with the necessary modifications in the process flowsheet to reduce the pollution to a target amount. It considers various ways to achieve the desired goal such as manipulation of process equipment, structural changes in the flow sheet, selection of the mass separating agent, configuration of the separation systems rerouting of streams and addition of new units and so on (Noureldin, 2000). One important aspect is that to reduce a particular pollutant from a waste stream it does not only confine to that stream rather it considers all the process streams which are somewhat connected to that component because it believes that pollution prevention is a multimedia problem (El-Halwagi, 1997). For selection of the mass separating agents for the separation process it emphasize to utilize the process derived stream which will be otherwise wasted. It also deals with the optimal matching of the waste streams and waste separating agents available in the process. In the literature mass integration technique is well demonstrated to minimize the water usage in process industries (Wang and Smith, 1994, 1995; Olesen and Polley, 1997; Feng and Seider, 2001; Hallale, 2002; Tan et al., 2002; Manan et al. 2004; Foo et al., 2006).

Therefore, mass integration provides a wide variety of alternatives to the process designers to improve the process performance from the pollution prevention viewpoint. To identify the mass integration opportunities Source-Sink mapping diagram could be used.

2.3.2.1 Source-Sink Mapping Diagram

Source-sink mapping diagram is a useful tool which represents graphically different sources and sinks in a flowrate vs. composition diagram. Source refers to the unit which is delivering the pollutant stream to the sink for the recycling and conversely sink is the unit which is receiving the pollutant or the waste material for the recycling. It maps all the sources and sinks that are relevant to a particular pollutant and hence, it provides a framework to investigate further about different P2 strategies for achieving the target.

This is quite useful in particular, for defining the recycling strategies of a pollutant, which include i) the decision about recycling without separation or with separation, ii) how much pollutant to recycle, iii) in case of separation, how much to separate and iv) strategies of mixing and segregation. It also determines how much of the target could be achieved using all sorts of the recycling strategies. In this way, indirectly it indicates how much of the target is required to be achieved through the source reduction strategies.

Figure 2.3 shows a typical source-sink mapping diagram, where all the sources and sinks for a particular pollutant is mapped. In fact, for all the units there have some design constraints regarding the range of flow rate and the composition of a particular component it can handle; so, the sinks are mapped based on that range. The sinks are mapped based on that composition and flowrate ranges and the source are mapped based on the composition and the flowrate data of the waste material. In the figure, extractor bottom, distillation bottom and the off-gas condensate are the sources and the absorber is mapped as a sink. Absorber can accept the composition of the concerned pollutant up to

21 ppm and the minimum and maximum flowrates that it can accept are 4 and 4.5 kg/sec. For the plant at the design level, this data could be obtained easily with the aid of the process simulation tools, therefore, in the present methodology the process simulation tool is also suggested which could be used standalone as discussed before or could be integrated with the source-sink diagram for data support. The figure shows that some sources stay on the right and some on the left of the sink's acceptable range. The source that is on the right of the sink cannot be directly recycled due to the higher in pollutants composition so in this case in order to recycle, separation is important to reduce the concentration to the acceptable limit. Similarly, the sources on the left can be directly recycled to the sink. In the figure, the pollutants composition in the distillation bottom and the off-gas condensate is higher as they stay on the right of the absorber's acceptable band, therefore, these two streams cannot be recycled directly without reducing the concentration to the acceptable limit via a separation operation. That separation operation if possible should be done with the aid of any process stream, otherwise suitable external mass separating agent could be used. Some sources may stay above the sink range and some below. It means that no sources match the sink flowrate requirement. Based on the relative position of the source and sink, one can decide the potential recycling strategies including mixing and segregation of the source streams.

As for example, in order to recycle off-gas condensate and the extractor bottom to the absorber, mixing with other stream is important. Similarly, in order to use the distillation bottom, it must be split in order to reduce the flowrate and composition to the acceptable limit of the sink.

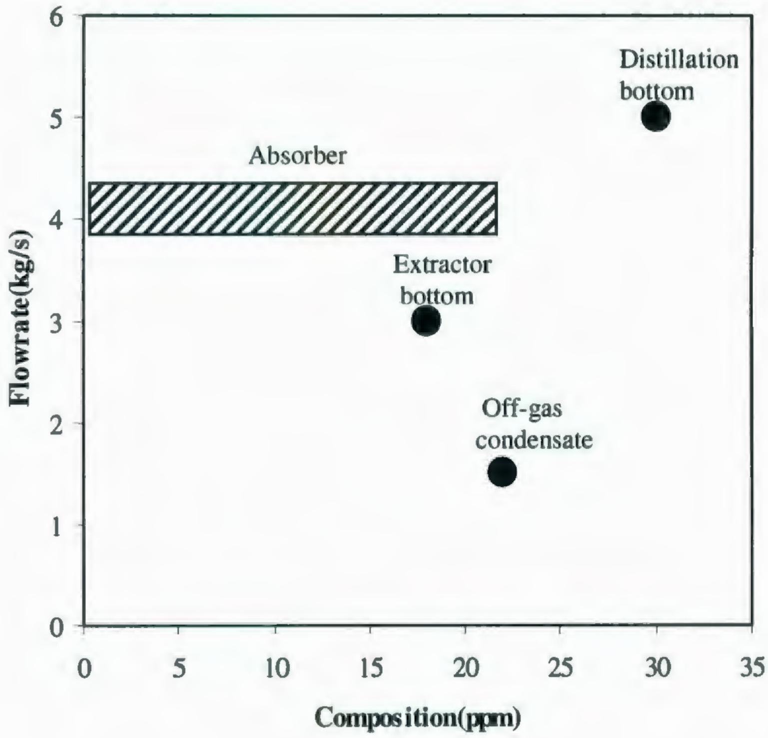

Figure 2.3: Typical Source-sink Mapping Diagram

2.3.3 P Graph

P graph is a tool which helps the designers to track the sources of the pollutants/waste generation. This provides a simple graphical basis to identify the areas where P2 opportunities are available. For drawing the P graph one needs to characterize the waste and identify the most toxic pollutants and the most significant waste materials. Then the components of concern are back tracked to examine their detailed pathway, i.e. where they are initially formed and their transport and fate throughout different processes up to the waste. This pathway is critically analyzed to find out the potential alternatives for addressing the pollutions. Figure 2.4 illustrates a simple p-graph. Here the product is C and the waste is D which is a toxic pollutant. In order to develop the possible pollution

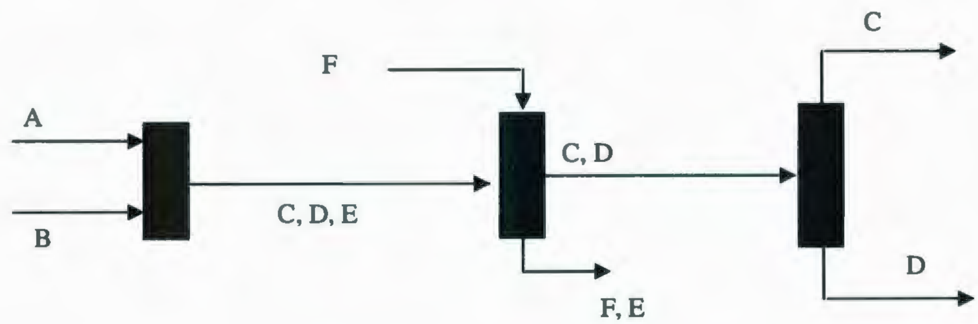

Figure 2.4: P-graph for Tracking of the Pollutant D

prevention strategy the designer needs to backtrack to see the all sources of D. The diagram shows that D is originating from the reactor as a byproduct, and then it is moving through the first separator and then separated finally in the distillation column. Therefore, in order to prevent the D, one can think about the possible modification in reaction mechanism by using recycle option or adding some additives to the reactor. Another option might be use of reactive distillation system to change the pollutant D. Each p-graph can be drawn for separate component, or one single p-graph could be used for all the components of concern.

The p-graph is conventionally used for the existing process where data for waste characterization and tracking is available. Therefore, it can not standalone work during the new flowsheet refinement. Process simulation tool along with the p-graph could provide necessary mass balance data and develop the p-graph at this level. P-graph can guide the designers where more attention needs to be paid for addressing the components of concern. However, it cannot provide the specific guidelines what changes will prevent the pollution.

2.3.4 Cause-and-Effect Diagram

When P-graph is drawn, the designers need to know what different source reduction options are available with the identified process unit, or stream to reduce the pollutants emission up to a desired level. At this level only, minor changes will be taken into account such as change in operating temperature, pressure and composition of the stream, changes in design parameters of the process unit, i.e. size of the reactor, size of the tray, number of staging etc. The complete cause-and-effect diagram will present all the options related to different units and streams in the entire flowsheet. The next step is to analyze the options with the help of the process simulation tool and they are subsequently evaluated to check the overall economic and environmental performance with the aid of the IPCP tool. The acceptable options are incorporated into the flowsheet for its improvement.

2.3.5 Process Simulation

Process simulation is used to model a wide variety of process operations and their interactions in initial design as well as retrofit stage (Pennington, 1997). It provides in-depth knowledge of process behavior and helps perform following tasks:

- Carrying out the mass and energy balance data at different operating conditions.
- Evaluation of different possible design options at conceptual stage.
- Selection of optimal plant configuration for achieving maximum productivity and minimal waste.
- Selection of optimal operating conditions for producing minimum waste.
- Monitoring the effect of source and sink manipulation on plant emissions.
- Performing the cost analysis of a plant.

A number of process simulation tools are commercially available such as Aspen HYSYS, ASPEN Plus, ChemCad, PRO etc. Some of them are capable of studying the dynamic process simulation, which helps optimize the control parameters, and examine the possible effects of equipment sizing and external disturbances such as operating parameters change, compositional change on plant operations. From pollution prevention aspect, dynamic simulation can be used to get the reduced emissions via optimum equipment sizing and help estimate the peak emissions and energy demands.

Therefore, process simulation is a powerful way to investigate the pollution prevention opportunities during process design as well as the retrofit stage. It helps evaluate the different pollution prevention strategies, such as in-process recycling, stream segregation, rerouting etc. by providing plant energy and mass balance data. However, it does not systematically guide the designer on which strategy will reduce the pollution (Pennington, 1997), thus, the success of the standalone use of simulation tool greatly depends on the intuition of the designer and it may waste a significant amount of time and effort.

2.4 Life Cycle Assessment: This has been discussed in section 3.4 of manuscript chapter 3 and will not be discussed here, however the framework of the life cycle approach is described below.

2.5 Life Cycle Assessment Framework

The general methodological framework for LCA developed by SETAC, is internationally accepted (Khan et al., 2004). The international standardization organization (ISO) also independently developed the framework for LCA (Azapagic, 1999). Both comprise four main phases; the first three phases are identical, however, the only difference noted in the last phase. In the SETAC framework, the last phase involves improvement assessment while in the ISO framework it is termed as interpretation, which in broad sense is very close to improvement assessment (Azapagic, 1999). Figure 2.5 shows different steps of lifecycle assessment developed by SETAC (Fava et al., 1991).

2.5.1 Goal and Scope Definition

This defines the system boundaries for the assessment of the products, process or activity, details accuracy and data quality, and impact models to be used for the analysis (Fava et. al., 1991). The system functions are specified and expressed in terms of functional unit. In setting the system boundaries, it is useful to differentiate between the foreground and background systems (Clift et al., 1998). The foreground systems involve the processes directly associated with the investigated process, product or activity, while background systems embody all the processes and related activities for supplying energy and materials input to the foreground systems (Azapagic, 1999).

Figure 2.5: Life Cycle Framework

2.5.2 Inventory Analysis

This involves the quantification of environmental burdens over the defined system boundary of a process or activity (ISO, 1997 (14041)). Environmental burden accounts for any releases of contaminants that have potential adverse impacts on environment. It quantifies the emissions to air water and soil, energy usage and materials consumption. The collected data must be related to the functional unit (ISO, 14041, 1997).

2.5.3 Impact Assessment

The inventory data is very difficult to compare and interpret, therefore the LCA frameworks considered impact assessment to be an essential part of life cycle analysis (ISO, 14042.3 (1998), Fava et al., 1991) followed by the inventory analysis phase. It consists of three steps: i) classification and characterization ii) normalization and iii) evaluation. Figure 2.6 shows systematically different steps of impact assessment. The steps are depicted below.

2.5.3.1 Classification and Characterization

In classification step all the inventory data are classified according to their effects. For instance, classification of the emissions to air, water and soil, sorting of the air pollutants in accordance with global warming, ozone layer depletion etc. The risk of different emissions is calculated for each effect category. In this characterization step most of the earlier research calculated the probable effects due to the emissions over global, continental or regional boundary (Goedkoop et al, 2004), however local impact is not considered.

2.5.3.2 Normalization

In this step different calculated effects are compared on a common scale in order to get better understanding of the relative size of an effect. Normalization results in a set of effect scores which have same or no dimension (Goedkoop and Spriensma, 2001). The reference value used for normalization is not fixed, a number of reference values can be used. A commonly used reference value is the average environmental load per year of an inhabitant in a specific country or region (Goedkoop et al., 2004). Other reference values are also used in different methods (Brentrup et al., 2004, Goedkoop et el, 1995, Wenzel et al., 1997). If assessment is based on a single effect category normalization step is eliminated (IPCC 2001, Frischknecht and Jungbluth, 2003).

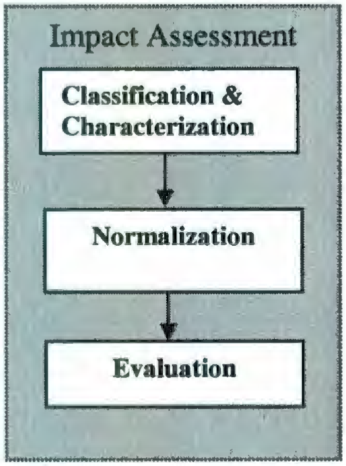

Figure 2.6: Different Steps of Impact Assessment Phase

2.5.3.3 Evaluation

Although normalization compares all the impact categories on a same scale, it does not inform anything about the relative importance of different impact categories. Therefore, normalization results cannot be used for final judgement. To resolve this problem different weighting factors are used among the impact categories. Usually normalized scores of each category are multiplied by a weighting factor, which are subsequently added to get an overall single score. According to the ISO 14042 weighting is an optional step of life cycle impact assessment. Some LCA methods did not use the weighting step (IPCC 2001, CMLCA, 2004), while others did use (Goedkoop et al 1995, Goedkoop and Spriensma, 2001, Steen, 1999, Wenzel et al., 1997). Weighting step can be eliminated for the cases when the normalized scores of an option become higher for all impact categories over other option or the assessment considers only one impact category (Goedkoop and Spriensma, 2001). It can also be dropped when the assessment aims to determine the total environmental burden over the entire life cycle.

Weighting is the most controversial step of the impact assessment (Goedkoop and Spriensma, 2001). Weighting factors have been determined in the literature based on any of the following principles: cost of health care, pollution preventing cost, the evaluation of experts, gap between the current impact level and target level, actual damage or analytical hierarchy of the impact categories (Goedkoop et al., 1995).

2.5.4 Improvement Assessment

In this phase the most significant impact sources are identified and the possible alternatives and or/modifications to reduce the pollution are systematically evaluated (ISO-14043).

2.6 Impact Assessment Methods: For impact assessment several methods have been developed, some common approaches are WAR algorithm, Eco-indicator 95 and 99, Ecopoints 97 and EPS 2000. These are discussed in the following sections.

2.6.1 WAR Algorithm

This approach has been briefly discussed in section 3.1 of Chapter 3; however, here it is described in more detail to assist the readers.

WAR algorithm stands for Waste Reduction Algorithm. It has introduced an environmental assessment technique for evaluating different process designs from the view of pollution prevention. It was first introduced by Hilaly and Sikder (1994). It is a methodology that allows tracking of the pollutants throughout the process with the aid of pollution balance. Afterwards Cabezas et al. (1997) amended this concept to introduce potential environmental impact balance (PEI) instead of pollution balance. The potential environmental impact is a conceptual quantity that cannot be directly measured, however one can calculate PEI from related measurable quantities using functional relation between the two. The WAR algorithm is based on the impact conservation equation and it quantifies the impact of the pollutants throughout the process. The impact conservation equation is as follows:

$$DI_{syst}/dt = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen} \tag{2.7}$$

Where, I_{syst} is the potential environmental impact content inside a process, $\dot{I}_{in}$ is the input rate of impact, $\dot{I}_{out}$ is the output rate of impact, and $\dot{I}_{gen}$ is the rate at which impact is generated in the system by chemical reactions or other means. For steady state processes, the conservation equation reduces to:

$$0 = \dot{I}_{in} - \dot{I}_{out} + \dot{I}_{gen} \tag{2.8}$$

This implies that no potential environmental impact accumulates in the system.

In equation 1 and 2 only impacts due to the materials are considered, however in later version of WAR algorithm the impacts due to energy is included (Douglas and Cabezas, 1999). The impacts are measured related to the flow rate, composition and chemical specific overall environmental impacts.

The expression is as follows:

$$\dot{I} = \Sigma \dot{M}_i \Sigma X_{k,j} \psi_k \tag{2.9}$$

Where, $\dot{I}$ is the potential impact rate for stream j, $\dot{M}_j$ is the mass flow rate for stream j, X_k is the mass fraction of component k in stream j and ψ_k is the potential environmental impact of component k.

In WAR algorithm six potential environmental impact indexes are considered that characterize the PEI generated within the process and the output of PEI from the process. Potential environmental impact of each chemical to a particular category is calculated based on the potential hazard based score, which is normalized with the average hazard score of same category for a significant number of chemicals. WAR algorithm does not either use the overall single impact score for easy comparison of different P2 options or use the optimization technique to select the overall best P2 option. In WAR algorithm there is a lack of reasonably justified method to assign environmental weighting factors to different impact categories, which makes the overall impact index uncertain. As impact calculation is based on potential hazard value, in WAR algorithm all levels of pollutants are considered to have adverse environmental effects, which might incorporate uncertainty (Nourai et. al., 2001). Furthermore, WAR algorithm incorporates the gate-to-gate LCA, therefore the overall environmental friendliness of an option selected using WAR algorithm is questionable.

2.6.2 Ecopoints 97

The Swiss Ministry of the Environment (BUWAL) has developed the Ecopoint 97, a cradle-to-grave LCA approach for environmental impact assessment of different product design options. It considers the actual pollution and critical targets that are derived from Swiss policy. It is one of the earliest approaches for impact assessment with single score. Weighting of different effect categories is based on distance-to-target principle. The Ecopoints methodology does not use a classification. It assesses impacts individually. Although this allows for a thorough and very substance-specific method, it has the drawback that only a few impacts are assessed. For normalization Ecopoints system employs target values rather than current values. The Ecopoint system considers the policy levels rather than sustainability levels. Policy levels are usually a compromise between political and environmental considerations.

2.6.3 Eco-indicator 95 and 99

Eco-indicator 95 is a cradle-to-grave life cycle environmental impact assessment approach for product and process design, developed under the Dutch NOH program by PRé consultants. It is a damaged-oriented approach, it only takes account of the effects, which potentially damage human health and ecosystems. Therefore, the raw materials depletion and the space requirements for waste are not evaluated. Characterization factors are calculated at end-point level (damage). Normalization data is calculated on European level. The weighting factors are determined on the basis of distance-to-target principle, i.e. the distance between the current and target values of an effect. The basic assumption is that the seriousness of an impact can be judged by the difference between the current and a target level.

Eco-indicator 99 is the successor of Eco-indicator 95. In Eco-indicator 99, weighting is based on actual damage results rather than distance-to-target principle. The number of subjects to be weighted has been reduced to three to facilitate the panel of experts for providing meaningful weighting factors. For exposure analysis it employs multimedia fate and transport model, for effect analysis dose and response model and finally damage model is used to calculate the number of year life lost and the number of years lived disabled (Goedkoop et. al., 1995; Goedkoop and Spriensma, 2001).

2.6.4 EPS 2000

EPS is a cradle-to-grave impact assessment approach developed to assist the product developers for comparing two product options in order to find out which option has the least environmental impact. Five impact categories are considered: human health, ecosystem production quality, abiotic stock resource, biodiversity and cultural and recreational values (Steen, 1999). Empirical, equivalency and mechanistic models are used to calculate default characterization values. This method does not include the normalization step and weighting is made through valuation. Weighting factors represent the willingness to pay to avoid changes. The environmental reference is taken as the present state of the environment and the indicator unit is considered as ELU (Environmental Load Unit).

2.7 Fundamentals on Exergy Analysis

Exergy is the maximum theoretical work obtainable from a system (Moran, 2004). The maximum work is only possible when the system reaches both thermal and mechanical equilibrium with the surrounding. Therefore, the amount of work obtainable from a system depends on the surrounding conditions. The greater the difference between the system and its surrounding, the greater the work output from the system to surrounding (Ozturk et al. 2006). Energy can be conserved in any situation but exergy cannot be conserved without truly reversible process. Exergy is destructed by the irreversibility, whereas energy is not (Moran, 2004; Sengupta, 2007).

Exergy analysis can locate the processes/components important to be modified for improving the performance of a process or component through the evaluation of exergy destruction (Sengupta, 2007). Therefore, exergy analysis provides more realistic basis to improve the system's performance (Rosen, 2008), while the energy analysis cannot always do that and even sometimes provides misleading information. For example, energy analysis in a steam turbine plant shows that condenser looses a significant amount of energy indicating that condenser is a potential source for improvement. However, exergy analysis reveals that exergy loss in the condenser is very insignificant and it does not have any significant potential for the improvement. Similarly, energy analysis in a heat recovery steam generator (HRSG) of a combined cycle power plant shows that amount of energy that the hot flue gas gives up is gained by the feed water. This indicates that no energy loss occurs within the HRSG, and therefore, HRSG design improvement is not important. However, exergy analysis shows that a significant amount of exergy destruction occurs in the HRSG unit due to the irreversibility caused by the pipe friction and the heat transfer at finite temperature difference between the steam and feed water. This indicates that significant effort is required to put for the design improvement of HRSG in order to reduce the exergy destruction.

Due to the robustness of the exergy analysis over energy analysis, the applications of exergy analysis have been increasing continuously over last few years for the design and performance evaluation of thermal systems.

Ozturk et al. (2006) conducted an exergy assessment in a geothermal power plant by estimating exergy destruction in each component of the plant. They also performed parametric studies to find out the optimum operating conditions that resulted in the maximum exergy efficiency of the plant. Rosen and Tang (2007, 2008) carried out exergy analysis in a coal fired steam turbine power plant and noticed that that the highest exergy destruction occurred in the steam generator. This finding assisted them to reduce the irreversibility of the steam generator by reducing the amount of the excess combustion air to the steam generator. Sengupta et al. (2007) investigated the performance of a coal based thermal power plant at different loads and condenser pressures based on exergy analysis. The observations showed that the highest exergy destruction occurred in steam generator which was about 60%. At reduced load and higher condenser pressure the exergy efficiency of the plant decreased. Apart from these, in last few years, some other studies on exergy analysis in different thermal systems have also been reported (Martaj et al., 2006; Dadgas, 2005; Tyagi et al., 2005; Kopac and Zemher, 2004).

2.7.1 Exergy Components

The total exergy of a system E could be divided into four different components: physical exergy, E^{PH}, kinetic exergy, E^{KN}, potential exergy, E^{PT} and chemical exergy, E^{CH} (Bejan et al, 1996).

$$E = E^{PH} + E^{kN} + E^{PT} + E^{CH} \quad (2.10)$$

The sum of physical, kinetic and potential exergies is referred to thermo-mechanical exergy, E^{TM}, which could be defined as the maximum theoretical work obtained from a system when it comes into thermal and mechanical equilibrium with the environment. Therefore, exergy has two major parts: Thermo-mechanical part and chemical part.

$$E = E^{TM} + E^{CH} \quad (2.11)$$

Physical exergy of any closed system at a particular state can be given by the following expression

$$E^{PH} = (U - U_o) + p_o\,(V\text{-}V_o) - To\,(S\text{-}S_o) \quad (2.12)$$

Specific exergy is the exergy per unit mass, e, so, specific physical exergy is:

$$E^{PH} = (u - u_o) + p_o\,(v\text{-}v_o) - T_o\,(s\text{-}s_o) \quad (2.13)$$

Total specific exergy could be expressed as:

$$e = (u + V^2/2 + gz - u_o) + p_o\,(v\text{-}v_o) - T_o\,(s\text{-}s_o) \quad (2.14)$$

u and v and s denote internal energy and volume and entropy of the system for unit mass. V, T, p and z denote respectively, velocity, volume, temperature, pressure and elevation of the system at a specific state. u_o, v_o, so refer to the values of the same properties when the system reach equilibrium state.

2.7.2 Exergy of Open System

Exergy of any open system or flow exergy can be described by the following expression:

$$e_f = h - h_o - T_o\,(s-s_o) + V^2/2 + gz \qquad (2.15)$$

Where h and h_o refer to the enthalpy values per unit mass at a specified and reference states.

Exergy change between two states can be given by:

$$ef_1 - ef_2 = h_1 - h_2 - T_o\,(s_1-s_2) + (V1^2 - V2^2)/2 + g\,(z_1-z_2) \qquad (2.16)$$

2.7.3 Chemical Exergy

Chemical exergy could be defined as the maximum theoretical work that could be obtained from a system due to the variation of concentration of any components at reference temperature and pressure with respect to its concentration in the reference environment.

If any hydrocarbon C_aH_b at T_o,p_o reacts with O_2 and form a moles of CO_2 and b/2 moles of water the exergy of the fuel could be calculated using the following formula:

$$\bar{e}_F^{ch} = \left[\bar{g}_f + \left(a+\frac{b}{4}\right)\bar{g}_{O_2} - a\,\bar{g}_{CO_2} - \frac{b}{2}\bar{g}_{H_2O(l)}\right](T_o, p_o) + a\,\bar{e}_{O_2}^{ch} + \left(\frac{b}{2}\right)\bar{e}_{H_2O(l)}^{ch} - \left(a+\frac{b}{4}\right)\bar{e}_{O_2}^{ch} \qquad (2.17)$$

$\bar{g}$ refers to the Gibbs functions for different reactants and $\bar{e}_F^{ch}$ refer to the chemical exergy values for different reactants and products. The standard chemical exergy values for different components are available from chart (Appendix A). Two different models are used for calculating the exergy values and the value for a particular component varies across the models. The exergy of fuel also could be calculated using the following equation:

$$\bar{e}_F^{ch} = \left[\bar{h}_f + \left(a+\frac{b}{4}\right)\bar{h}_{O_2} - a\bar{h}_{CO_2} - \frac{b}{2}\bar{h}_{H_2O}\right] - T_o\left[\bar{s}_f + \left(a+\frac{b}{4}\right)\bar{s}_{O_2} - a\bar{s}_{CO_2} - \frac{b}{2}\bar{s}_{H_2O}\right] \quad (2.18)$$

Here, $\bar{h}$ refers to heat of formation and $\bar{s}$ refers to absolute entropy of different reactants and the products. The above two formulas also could be used if fuel combustion contains other components, such as NOx, SOx, CO etc. In such case, the reaction should be balanced first and then the above formulas should be modified depending on the number of products.

2.7.3.1 Chemical Exergy of Ideal Gases

Consider any pure gas is at temperature and pressure T_o, p_o, it can be isothermally expanded to the pressure $y^e p_o$ and thus some theoretical work could be obtained due to this isothermal expansion. y^e is the mole fraction of the gas at the reference environment, the chemical exergy of a gas increases with the decrease of the value of y^e. The chemical exergy of any pure gas could be quantified by the following expression:

$$e^{ch} = \bar{R}T_o \ln\left(\frac{1}{ye}\right) \quad (2.19)$$

2.7.3.2 Chemical Exergy for an Ideal Gas Mixture

For an ideal gas mixture, chemical exergy could be quantified by the following equation:

$$e^{ch} = \sum_i y_i e_i^{ch} + \bar{R} T_o \sum_i y_i \ln y_i \qquad (2.20)$$

y_i and e_i^{ch} refer to the mole fraction and chemical exergy of each component of the gas mixture.

2.8 Exergy Balance Equation

At steady state, ideally the rate of exergy enters to a control volume must be equal to the rate of exergy leaving from it, if the control volume has single inlet and exit, the exergy rate balance equation could be written as follows:

$$0 = \sum_j \left(1 - \frac{T_o}{T_j}\right) Q_j - \dot{W}_{cv} + \dot{m}\left(e_{f1} - e_{f2}\right) - \dot{E}_d \qquad (2.21)$$

Where, $\dot{m}$ is the mass flowrate, $\sum_j \left(1 - \frac{T_o}{T_j}\right) Q_j$ is the exergy accompanying heat, $\dot{W}_{cv}$ is the exergy in the form of work. j is the number of stream through which heat is transferred from the system. In reality, no process is reversible and therefore, some entropy is generated due to the irreversibility and a significant amount of exergy is destructed, which is quantified as $\dot{E}_d$. Exergy destruction per unit mass is denoted as $\dot{e}_d$.

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Chapter 3

Sustainable Development of Process Facilities:

State-of-the-art Review of Pollution Prevention Frameworks

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Preface

This manuscript chapter presents a state-of-the-art literature review on the existing pollution prevention approaches and finally proposes a holistic approach for pollution prevention addressing some of the limitations of the existing approaches. A version of this paper has been published in the *Journal of Hazardous Materials* (Hossain et al., 2008).

The principal author (Khandoker Hossain) received the motivation of pollution prevention research from the co-authors (Drs. Khan and Hawboldt), who assisted the principal author in conceptualizing the pollution prevention through helpful discussions and by providing materials support. The principal author actively participated in extensive literature review, concept development, identification of challenges, problems formulation, as well as designing the framework of the P2 approach. In addition, he also conducted a qualitative case study and wrote the first draft of this manuscript. The co-authors reviewed the proposed approach and the manuscript and provided valuable suggestions and corrections.

Abstract

Pollution prevention (P2) strategy is receiving significant attention in industries all over the world over end-of-pipe pollution control and management strategy. This paper is a review of the existing pollution prevention frameworks. The reviewed frameworks contributed significantly to bring the P2 approach into practice and gradually improved it towards a sustainable solution, nevertheless some objectives yet to be achieved. In this context, the paper has proposed a P2 framework 'IP2M' addressing the limitations for systematic implementation of the P2 program in industries at design as well as retrofit stages. The main features of the proposed framework are that firstly, it has integrated cradle-to-gate life cycle assessment (LCA) tool with other adequate P2 opportunity analysis tools in P2 opportunity analysis phase and secondly it has reused the risk-based cradle-to-gate LCA during the environmental evaluation of different P2 options. Furthermore, it multi-objective optimization phase, it simultaneously considers the P2 options with available end-of-pipe control options in order to select the sustainable environmental management option.

Keywords: Pollution Prevention, Life cycle assessment, P2 framework, P2 evaluation

1.0 Introduction

Until recently end-of-pipe pollution control and management was the major practice in most of the industries to reduce the pollutants emissions, however this is not a sustainable solution in the long term. It requires large infrastructure and manpower, which can be costly if not implemented properly (Nourai et al., 2001; Hilson, 2000; Warren et al., 1999). Therefore, presently governments, environmental legislators and researchers are focusing more towards the implementation of pollution prevention techniques, where the pollution is prevented before its generation (O'Malley, 1999; USEPA 1990; CEPA, 1999). P2 is an important part of the environmental management system (EMS), which does not deal with offsite recycling, energy recovery, treatment, and disposal. According to the US pollution prevention act, pollution prevention means "source reduction and other practices, which reduce or eliminate the creation of pollutants" (USEPA, 1990). It is suggested to achieve through: equipment or technology modifications, process or procedure modifications, reformulation or redesign of products, substitution of raw materials, and improvements in housekeeping, maintenance, training, or inventory control. The federal government of Canada defines pollution prevention as the use of "processes, practices, materials, products, substances or energy that avoids or minimizes the creation of pollutants and waste and reduces the overall risk to the environment" (CEPA, 1999).

P2 has substantial benefits over end-of-pipe pollution control and management. Apart from the reduced production cost, improved competitiveness, enhanced customer trust, improved environmental performance, and worker health and safety benefits, it conserves energy and materials through their optimal utilization (OECD, 1995). Industries are the major sources of pollution, therefore, the implementation of an effective pollution prevention methodology can lead to a cleaner and healthier environment. Some researchers and environmental organizations such as the US Environmental Protection Agency (EPA) and Environment Canada have developed pollution prevention frameworks to be used in industries. These frameworks have gradually improved the P2 methodology towards sustainable solutions. Nevertheless, some limitations and ambiguities are still prevailing, which need to be addressed. Therefore, a significant research is warranted in this area.

This paper reviews available pollution prevention frameworks and finally proposes a systematic and sustainable pollution prevention methodology 'IP2M'. The proposed methodology is built with risk based life cycle assessment and also includes health and safety as an important parameter for P2 option selection. It is applicable to process and allied industries at early design stage as well as during any modifications to existing industries.

2.0 Review of the Existing P2 Frameworks

In the literature, pollution prevention is sometimes termed as waste reduction, source reduction, waste elimination or waste avoidance (Fromm et al., 1986). The basic elements of pollution prevention are source reduction and in-process recycling (ENR, 1992). On the other hand, waste minimization usually includes the pollution prevention with off-site recycling (DOE, 1996). As pollution prevention is the preferred option of waste minimization, therefore, some waste minimization framework could also be used for practicing the pollution prevention in industries.

2.1 Frameworks Developed by the US EPA

The US EPA contributed in the early development of different pollution prevention frameworks. These frameworks are being practiced in the United States since the pollution prevention act has been approved. Depending on the context of different organizations and applications, these frameworks have been slightly revised. The summary of the frameworks is briefly described below.

2.1.1 Waste Minimization Framework

This framework was developed by the US EPA prior to the pollution prevention act and enforced the industries to implement the pollution prevention concept within their facilities. It has five major steps (Figure 3.1):

a) Planning and organization, which includes management commitment, setting of overall assessment program and organization of assessment program task force

b) Assessment phase, which mainly consists of data collection, prioritization of assessment phase, reviewing data and impact site, option generation, and screening and selecting the option for further review

c) Feasibility analysis phase based on technical and economic evaluation

d) Report preparation on assessment

e) Implementation

As an initial attempt, the framework provided an excellent basis for describing the basic phases of waste minimization. The main limitation of the framework is that during the feasibility analysis of different pollution prevention options it considers only the technical and economic evaluations, leaving other important parameters such as health and safety.

2.1.2 Facility Pollution Prevention Framework

The facility pollution prevention framework was developed by the US EPA in 1992 to help small to medium-sized production facilities to establish broad-based, multimedia pollution prevention programs in all business and geographic areas. It describes how to identify, assess, and implement opportunities for preventing pollution and how to stimulate the ongoing search for such opportunities. It consists of a series of sequential phases: i) establish the pollution prevention program, ii) organize program, iii) do preliminary assessment, iv) write program plan, v) do detailed assessment, vi) define pollution prevention options, vii) do feasibility analysis, viii) write assessment report, ix) implement the plan, x) measure the progress, and xi) maintain pollution prevention program (Figure 3.2). Compared to the previous framework, this framework is more detailed and suggests conducting the pollution prevention opportunity assessment in two steps rather than one-step assessment. The first phase

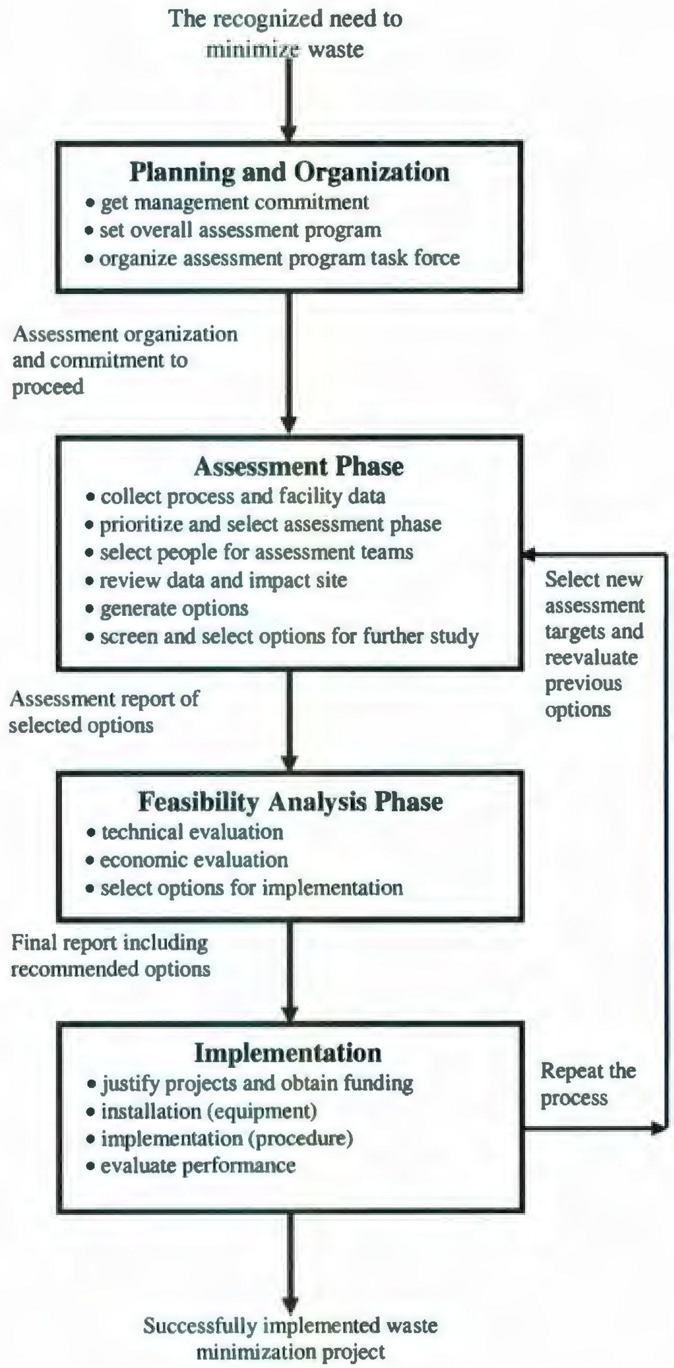

Figure 3.1: Waste Minimization Framework (EPA, 1988)

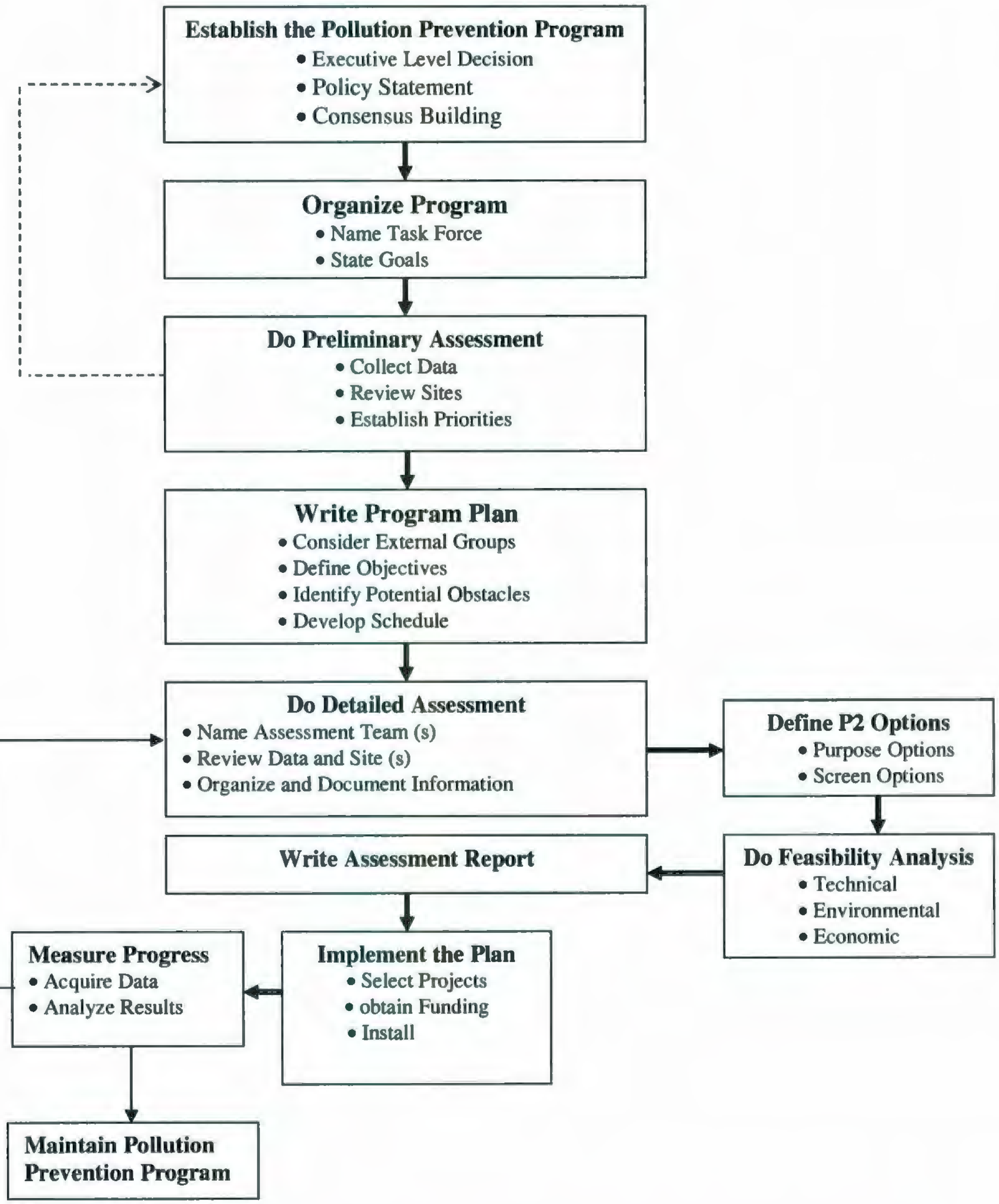

Figure 3.2: Facility Pollution Prevention Program Overview (EPA, 1992)

of the framework i.e. establishment of the pollution prevention program needs to be reviewed based on the feed back of preliminary assessment. Furthermore, in feasibility analysis phase, it includes the environmental objective apart from the technical and economic objectives, which would lead to the adequate selection of an overall environmental friendly option. To make a sound environmental evaluation, it is suggested that the information should be collected on the environmental aspects of the relevant product, raw material or constituent part of the process. This information would consider the environmental effects not only of the production phase and product life cycle but also of extraction and transportation of the raw materials and of treating waste. During the environmental evaluation, energy consumption should also be considered in the whole life cycle.

2.1.3 State of Ohio EPA Pollution Prevention Framework

In 1993, the Ohio EPA has introduced a pollution prevention framework, which is applicable to the reduction of all waste regardless of environmental media, quantity, or toxicity. It is a revised version of the US EPA facility pollution prevention framework. It has one additional step namely 'cost considerations' as compared to the facility pollution prevention framework, which has come just before the feasibility analysis phase (Figure 3.3). The most significant difference between the two frameworks is that in feasibility analysis phase, the US EPA framework suggests conducting a technical feasibility analysis first, then environmental and finally an economic feasibility. This gives more priority to environmental interest over economics.

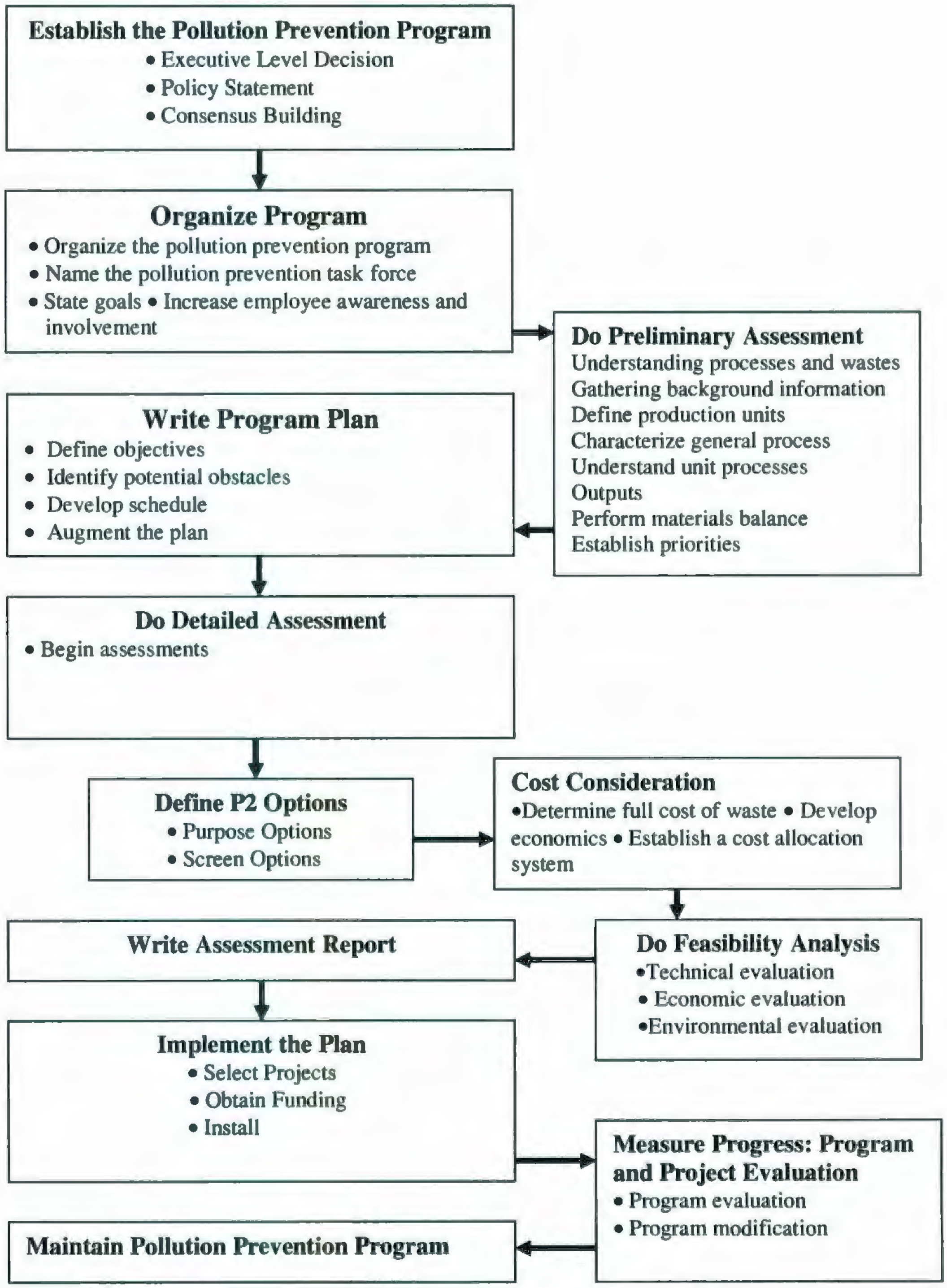

Figure 3.3: Ohio EPA Pollution Prevention Framework (Ohio EPA, 1993)

However, in the Ohio EPA framework economic feasibility has been given more importance over the environmental interest, so environmental evaluation has been considered as the last objective. It indicates that if economic feasibility fails then there is no need to proceed for the environmental evaluation for a particular P2 option. In the 'progress measuring phase', if the progress is not satisfactory then the US EPA facility P2 framework suggests repeating all the steps starting from the detailed assessment step. However, the Ohio EPA framework does not give any specific guidelines in this situation.

2.1.4 Limitations of the EPA Frameworks

The conceptual frameworks developed by the EPA provide the guidelines for implementing the pollution prevention from the initial stage to final stage, which is broadly accepted in different industries across the US as well as some other countries. Nonetheless, they have one common limitation in the feasibility analysis phase of P2 options. The feasibility analysis is done sequentially based on different criteria such as technical, environmental, economic etc. If any P2 option does not become feasible with respect to a particular objective function then it is not proceeded for further evaluations. Furthermore, in the P2 assessment phase the frameworks do not give any specific guidelines about which different engineering tools are to be employed and how. In feasibility analysis phase, risk and process safety issue is not considered.

The frameworks do not use multi-criteria optimization, which might not lead to an adequate selection of P2 option. They also do not provide any solutions if none of the P2 options are feasible.

2.2 Modification of the EPA Frameworks

2.2.1 Modification by Patek and Galvic

In order to address the limitations of the EPA frameworks, Petek and Galvic (1996) suggested some modifications to the EPA waste minimization framework. The first modification involves the use of some potential tools for P2 opportunity identifications, which include mass and energy balance, thermodynamic analysis, analysis of steam distribution, utilization and condensate system. This phase has been added after the assessment phase. Secondly, it adds a multi-criteria optimization tool after the feasibility analysis phase, which would help in selecting the overall best option based on multi-criteria evaluation.

2.2.2 Modification by the Environment Canada

The Environment Canada is using the facility pollution prevention framework of the US EPA with only one modification. It has added one additional step namely 'information gathering' in between the 'preliminary assessment' and 'writing of program plan' phase. The modification does not make any significant difference.

2.3 Other Existing Frameworks

The US Congress Office of Technology Assessment (OTA) has identified five broad areas of pollution prevention: i) in-process recycling, ii) process technology and equipment, iii) plant operations, iv) process input, and v) end product. In-process recycling involves the potential wastes or their components to be returned for reuse within the existing operation. Process technology and equipment incorporates changes in the basic technology and production equipment including modernization, modification or better control of process equipment. Plant operations include better predictive and preventive maintenance, better materials handling, improved process automation, separation of waste stream, increased use of sensors to detect and prevention of the non-routine waste. Process input involves the change in raw materials with different specifications and end product deals with changes in design composition or specifications of end products. In order to select the technically and economically feasible pollution prevention technique they have suggested conducting an adequate waste audit. However, no information is provided about how the waste audit alone can help select the appropriate pollution prevention opportunities (OTA, 1986).

Douglas (1992) has performed a hierarchical decision procedure that provides a simple technique for pollution prevention at the early stage of the design. The procedure consists of eight phases: type of problem, input-output structure of the flow sheet, recycle structure of the flow sheet, specification of the separation system, energy integration, evaluation of the alternatives, and preparation of flow sheet at each level to identify the waste generated.

Berglund and Lawson (1992) proposed that successful pollution prevention needs eight aspects to be considered at the early stage of a plant design: i) product design, ii) process design, iii) plant configuration, iv) information and control system, v) human resources, vi) research and development, vii) the supplier's role and relationship, and

viii) organization. They proposed three phases, the first phase includes good operating practice, waste segregation and simple recycling. The second phase is related to the addition or modifications of equipments and process modifications and control. The third phase is associated with more complex recycle and reuse techniques and changes in process by substituting raw materials, catalysts, product, etc.

These frameworks partially contributed to the implementation of P2 in process industries. However, they could not provide complete guidelines for practicing it in the real world. They also did not give any information about different objective functions that need to be considered. Furthermore, some important elements of P2 program such as management and employee's role, and P2 progress monitoring were overlooked.

2.3.1 Site Specific Frameworks

The US Department of Energy (1996) developed a P2 framework named 'P2DA' for the implementation of P2 at early design stage of a plant (DOE 1996). The framework is shown in Figure 3.4. It has six major steps: 1) planning and organization, 2) characterize of waste emissions, 3) establish strategy, 4) identify pollution prevention design opportunities, 5) analyze pollution prevention design opportunities, and 6) document results. The design assessment is carried out using facility life cycle assessment. For P2 opportunities identification, it employs a 'P2-edge' tool besides some traditional techniques such as brainstorming sessions, cause/effect diagrams, nominal group techniques, and benchmarking the best practices, and technologies of industry. The selection of the best environmental opportunity is mainly based on the

Planning and Organization
• Organize team • Budget and schedule the P2DA
Step 1 – Characterize Waste Streams
• Identify anticipated streams (construction, operations, closure/ dismantlement) • Quantify streams: source (unit operation/activity), regulatory status, expected frequency/duration/volume, unit cost, total cost
Step 2 – Establish Strategy
• Prioritize streams • Set boundaries for remainder of P2DA • Establish goals
Step 3 – Identify Pollution Prevention Design Opportunities
• Brainstorming techniques • Using P2- EDGE • Benchmarking Successful Techniques/Lessons Learned • Establishing design strategies
Step 4 – Analyze Design Alternatives
• Cost Analysis • Environmental Anaysis • Select P2DOs to implement
Step 5 – Document Results
• Implement Selected P2DOs into design • Measure progress/reevaluate goals • Generate P2DA Summary Report • Schedule follow up P2DA

Figure 3.4: Basic Framework for P2DA (DOE, 1996)

cost analysis, which considers the gate-to-gate life cycle rather than complete cradle-to-grave life cycle.

The Illinois Department of Energy and Natural Resources (ENR, 1992) has proposed a conceptual framework for implementing the pollution prevention program. The framework as shown in Figure 3.5 comprises the following major phases:

1. Obtaining support from top management
2. Getting the program started by beginning to institutionalize the process
3. Characterizing the process
4. Identifying potential pollution prevention opportunities for the facility
5. Determining cost of current waste generation and establishing a system of proportional waste management charges for those departments that generate waste
6. Selecting the best pollution prevention options for the company and implementing these choices.
7. Evaluating the pollution prevention program on a company-wide basis as well as evaluating specific pollution prevention projects
8. Maintaining the pollution prevention program

This framework considers the evaluation of different pollution prevention opportunities based on the separate evaluation of cost and technical criteria. The feasibility of any P2 options is determined by comparing with the baseline data. The different P2 options are ranked in terms of the environmental benefits and

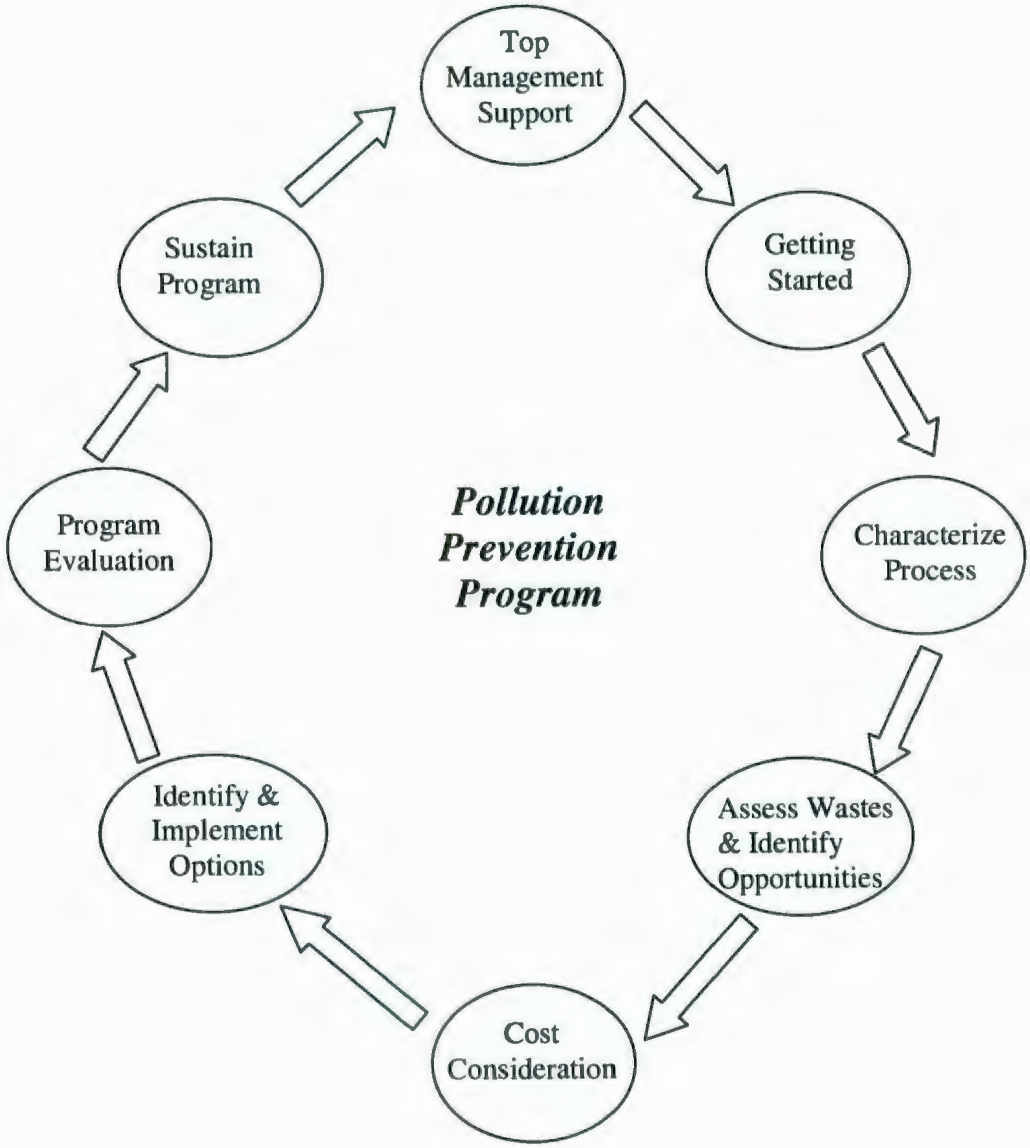

Figure 3.5: Pollution Prevention Loop (ENR, 1992)

subsequently the cost and technical parameters are evaluated. If the top ranked option becomes feasible then it goes for implementation, otherwise the feasibility of the next option is checked similar to the EPA approaches.

Noureldin and El-Halwagi (1999) have proposed a hierarchy of P2 strategies, which have three phases: no cost/low cost strategies, moderate cost modifications and implementation of new technologies (Figure 3.6). The first phase involves stream segregation or mixing, recycles and changes in operating conditions. Moderate cost modifications include the addition or replacement of equipment and substitution of materials such as solvent, catalyst, etc. Implementation of new technologies includes the use of environment benign chemistry, new processing technology etc. The significant contribution of the framework is that the analysis of P2 opportunities is conducted by employing mass integration strategy (MIS). MIS uses the concept of global flow of mass within the process to identify performance targets and optimize the allocation, separation and generation of streams and species (El-Halwagi, 1997; El-Halwagi and Springs, 1998). According to this P2 methodology, the acceptability of options is higher for no cost/low cost strategies and lower for new technologies and acceptability is based mainly on cost and environmental impacts. It indicates that cost has linear relationship with environmental impact i.e. as the cost of the modifications is higher the environmental impact of such modifications assumed to be better. Therefore, the same weight is applied to cost and environmental impact for accepting the P2 opportunities, which sometimes may give a misleading result.

One common limitation of the above three frameworks is that the evaluation is based on the site-specific data i.e., it is confined to the narrow system boundary, which only includes the manufacturing or processing site. Therefore, during raw material substitution or environmental impact evaluation it does not consider the cradle-to-gate or cradle-to-grave life cycle of the process/material. This might not lead to the selection of the best practicable process, the best available technology (BAT) and materials in terms of environment, health, and safety benefits.

2.3.2 Frameworks Based on Life cycle Assessment

Life cycle assessment can be used for environmentally benign product and process design. Azapagic (1998) has proposed a methodology for process design based on the life cycle assessment (Figure 3.7). The methodology uses LCA throughout the design process and thereby environmental consideration has been incorporated from the early design stage. The system boundary has been extended to include the quantitative evaluation of life cycles of different technologies and raw materials. The framework suggests that the process selection should be based on the optimization of a number of objectives apart from the technical, economic and environmental objectives, which includes suppliers and consumers requirements, legislative requirements, performance and materials etc. The limitation of the framework is that the optimization of a large number of criteria is practically very difficult and would result in a tremendous computational load. As all criteria cannot be given higher importance, therefore, such optimization increases the complexity without making much improvement in the results. A similar approach of integrating LCA with the conventional process deign framework has been proposed by Pistikopoulos et al., (1996), Kniel et al., (1996), and Stefanis et al., (1995).

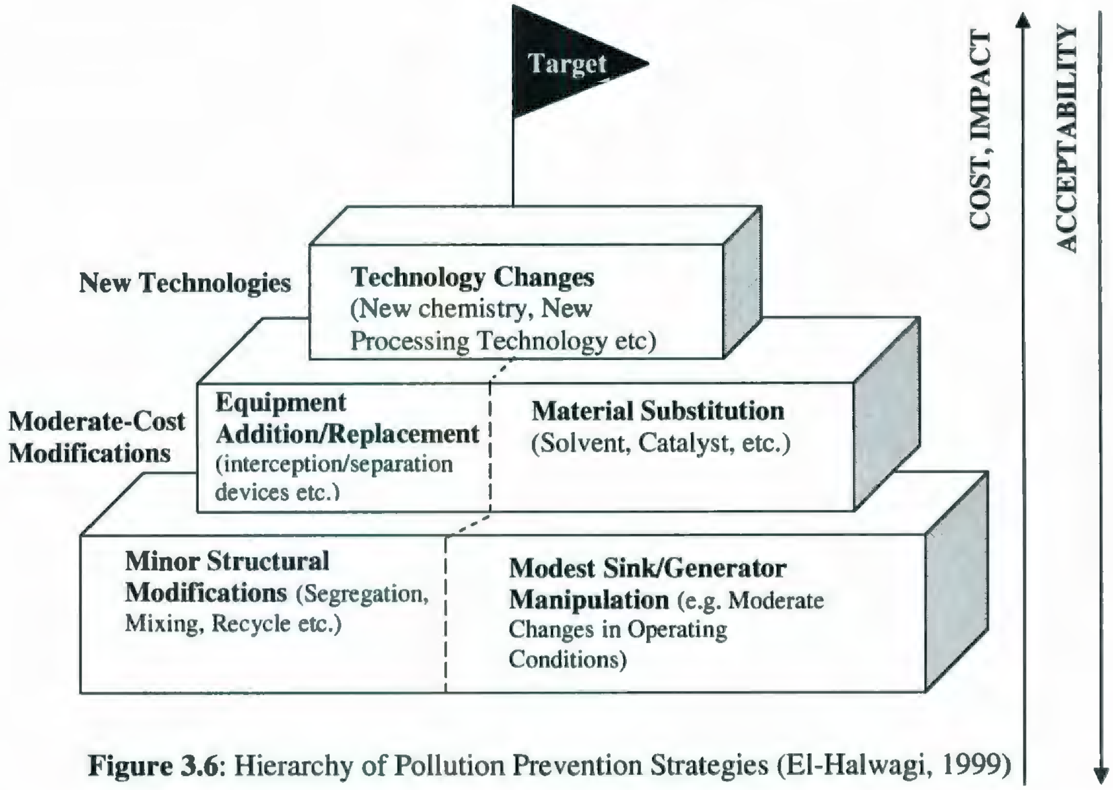

Figure 3.6: Hierarchy of Pollution Prevention Strategies (El-Halwagi, 1999)

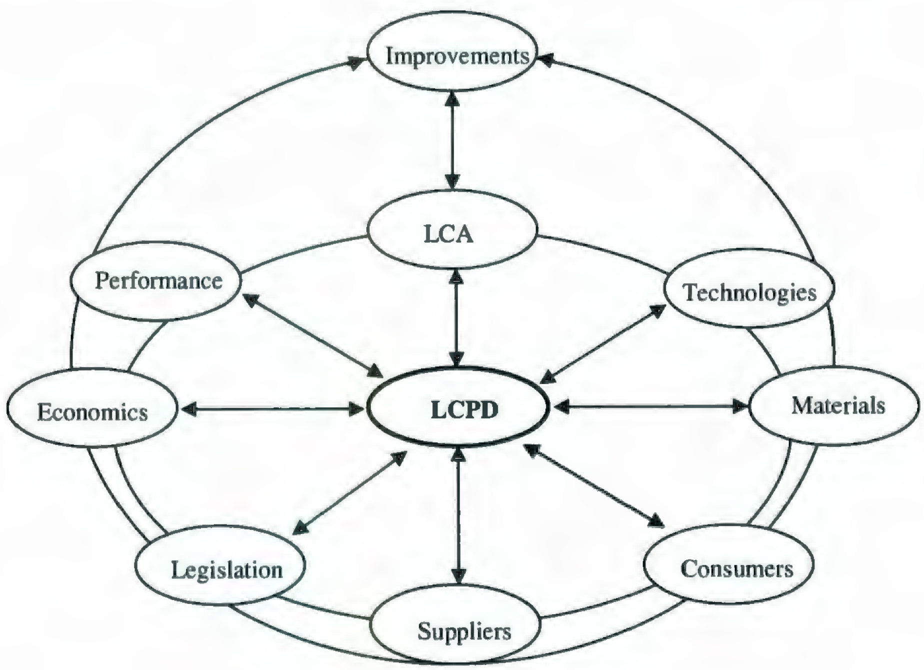

Figure 3.7: Methodological Framework for Life Cycle Process Design (Azapagic, 1998)

Khan et al., (2001) proposed GreenPro, a systematic methodology for process design. It considers minimization of environmental impact of a process by integrating the LCA technique within a normal process design and optimization framework (Figure 3.8). It used the LCA tool for assessing the environmental impact of a process or product through its complete life cycle. It proposed cost-effective process selection at the early stage of a plant design by employing the environmental objectives along with the technology and economics. The framework has integrated LCA with process modeling and multi-objective optimization tools. It enables optimal process design to reduce energy use and waste generation.

The above-discussed frameworks are mainly focused to the environmental friendly process design based on life cycle analysis at early design stage only. However, for process modification or redesign with the target of pollution prevention, P2 opportunity analysis tools are very crucial to be integrated with the LCA tool. In addition, the framework fails to provide the integrated solution of pollution prevention. Although initial design is an important stage of pollution prevention, pollution prevention opportunities need to be investigated in all stages/areas of plant design, operations and maintenance.

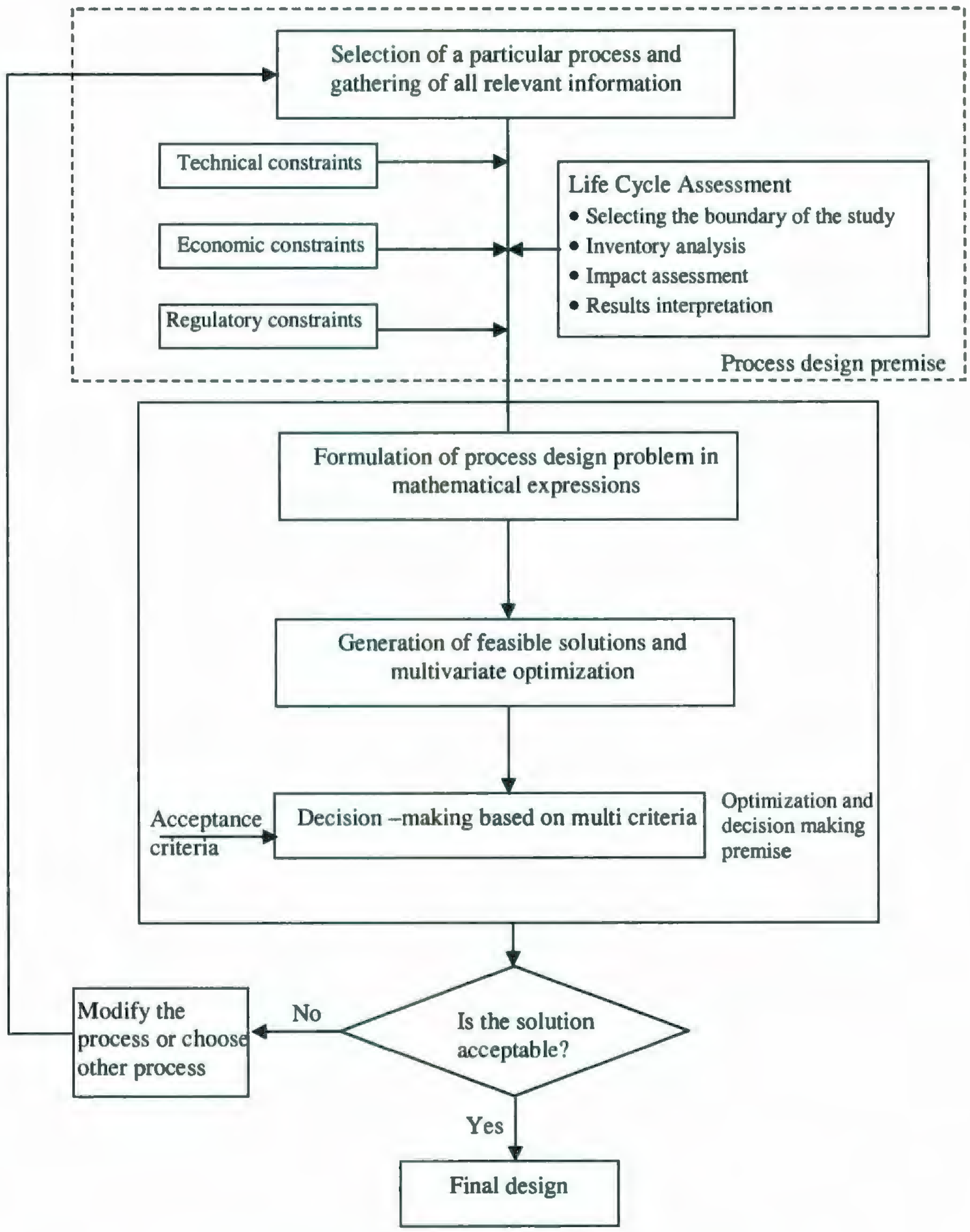

Figure 3.8: Basic Algorithm of Green Pro (Khan et al., 2001)

Table 3.1: Comparison of the Major Existing Frameworks

Framework	Comprehensiveness	P2 Opportunity Assessment Tools	Option Evaluation Criteria	Option Selection Criteria
Waste Minimization	Integrated (i.e. it integrates all the essential elements of P2 program)	Not mentioned in framework but LCA is suggested in the report body	•Technical •Economic	Priority based feasibility checking (PBFC)
Patek and Galvic	Integrated	HEN, MEN etc.	•Technical •Economic	Multi-objective optimization
EPA Facility	Integrated	LCA suggested in the report body	•Technical •Environmental •Economic	Priority based feasibility checking (PBFC)
US DOE	Integrated	Gate to gate LCA	•Economic •Environmental	Priority based feasibility checking
Illinois ENR	Integrated	Not mentioned	•Economic •Technical	Priority based feasibility checking
Noureldin and El-Halwagi (1999)	Only for process redesign/modification	Mass integration tool	•Economic	Lower cost more acceptable although environmental benefit is low
Azapagic (1998)	Only for initial process design	LCA is integrated with conventional process design framework	A number of criteria including technical, economic and environmental.	Multi criteria optimization
GreenPro	Only for initial stage process design	LCA is integrated with conventional process design framework	•Technical •Economic •Environmental	Multi-criteria optimization

3.0 Identification of Pollution Prevention Opportunities

Identification of the pollution prevention opportunities is the most important step of the P2 framework as the success in P2 program greatly depends on it. Significant research has been devoted to develop adequate tools or approaches to perform a quantitative environmental evaluation for identifying P2 opportunities. Some common tools are guide words techniques analogous to the HAZOP studies (Doerr, 1996; Potter and Isalski, 1992), mass and energy integration tools (Allen and Rosselot, 1997), graphical mass balance (Flower et al., 1993), process simulation (EPA, 1994; Nourai et al., 2000), WAR algorithm (Cabezas et al., 1999; Papalexandri et al., 1994), total site analysis (Dhole and Linnhoff, 1993), life cycle assessment (Clift and Longley, 1995) and net work synthesis technique (El-Halwagi and Manousiouthakis, 1989; Surivas and El-Halwagi, 1994a, Kiperstok and Sharratt, 1995; Wang and Smith, 1994; Kuo and Smith, 1998). Some of the important tools are briefly reviewed here.

3.1 WAR Algorithm

WAR algorithm stands for Waste Reduction Algorithm. It has introduced an environmental assessment technique for evaluating different process designs from the view of pollution prevention. It was first introduced by Hilaly and Sikder (1994). It is a methodology that allows tracking of the pollutants throughout the process with the aid of pollution balance. Afterwards Cabezas et al., (1997) amended this concept to introduce potential environmental impact balance (PEI) instead of pollution balance. The potential environmental impact is a conceptual quantity that cannot be directly measured, however, one can calculate PEI from related measurable quantities using functional relation between the two. The WAR algorithm is based on the impact conservation equation and it quantifies the impact of the pollutants throughout the process.

In WAR algorithm, six potential environmental impact indexes are considered that characterize the PEI generated within the process and the output of PEI from the process. Potential environmental impact of each chemical to a particular impact category is calculated based on the potential hazard based score, which is normalized with the average hazard score of the same impact category for a significant number of chemicals. WAR algorithm does not either use the overall single impact score for easy comparison of different P2 options or use the optimization technique to select the overall best P2 option. In WAR algorithm, there is a lack of reasonably justified method exists to assign environmental weighting factors to different impact categories, which makes the overall impact index uncertain. As the impact calculation is based on the potential hazard value, in WAR algorithm all levels of pollutants are considered to have adverse environmental effects, which might incorporate uncertainty (Nourai et. al., 2001). Furthermore, WAR algorithm incorporates the gate-to-gate LCA, therefore, the overall environmental friendliness of an option selected using WAR algorithm is questionable.

3.2 Mass Integration and Mass Exchange Networks

Mass integration is a holistic approach to the optimal allocation, generation, and separation of streams and species. It addresses pollution using a combination of strategies involving manipulation of process equipment, structural changes in the flow sheet, rerouting of streams and addition of new units (Noureldin, 2000). Mass integration has strong impact on process systems in terms of pollution prevention. It is based on the fundamental principle of chemical engineering combined with system analysis employing graphical and mathematical optimization based tools (El-Halwagi, 1997). The first step of conducting mass integration analysis is the development of a global mass allocation representation of the whole process from a species viewpoint. For each targeted species (e.g. each pollutant), there are sources and process sinks. Each sink/generator can be manipulated through design and operating parameters change. The sources must be prepared for the sinks through segregation and separation using mass exchange network (Garrison et al., 1995; El-Halwagi et al., 1996; El-Halwagi & Spriggs, 1996). Mass exchange network (MEN) synthesis is a combined synthesis and evolutionary design method (El-Halwagi and Manousiouthakis, 1989). It systematically optimizes considering the thermodynamic feasibility of mass exchange and economic evaluations to synthesize separation networks for achieving maximum possible mass exchange at minimal cost. In last few years significant numbers of research have been carried out in this area and consequently MEN concept is extended to a much wider range of problems. This includes the simultaneous synthesis of mass exchange and regeneration networks (El-Halwagi and Manousiouthakis, 1990); synthesis of reactive MEN (El-Halwagi and Srinivas, 1992; Srinivas and El-Halwagi, 1994); synthesis of combined heat and reactive MEN (Srinivas and El-Halwagi, 1994b); synthesis of waste-interception networks (El-Halwagi et al., 1996); heat-induced separation networks (Dunn et al., 1995; Dye et al., 1995; Richburg and El-Halwagi, 1995; El-Halwagi et al., 1995), water minimization problem (Wang and Smith, 1994, 1995; Dhole et al., 1996; Olesen and Polley, 1997; Sorin and Bedard, 1999; Polley and Polley, 2000; Bagajewicz, 2000; Dunn and Wenzel, 2001a,b; Feng and Seider, 2001; Hallale, 2002; Tan et al., 2002; Foo et al., 2003; Manan and Foo, 2003; Manan et al., 2004).

One serious limitation associated with the mass integration is that it only allows for reducing the ultimate concentration of the contaminants, however, they are not capable to address the pollutants considering the relative toxicity of each pollutant.

3.3 Total Site Analysis

Total site analysis is an approach for predicting the emissions of CO, CO_2, NO_x, and SO_x based on the correlation between energy use and pollutants emission (Dhole & Linnhoff, 1993). It can be used as a pollution prevention tool in certain applications despite the fact that it is not dedicated to environmental considerations. The limitation of the approach is that it is unable to predict the process-related emissions when they are not directly related to energy use and its applicability is very limited. Furthermore, it cannot identify upstream and downstream pollution sources related to a process system.

3.4 Life Cycle Assessment

Life cycle assessment (LCA) is a quasi-objective process for evaluation of the environmental loads caused by a product, process or single activity. The evaluation is obtained through quantification of the energy and materials consumption and wastes release into the environment. The assessment includes the entire life cycle of the product, process or activity encompassing extraction and processing of raw materials, manufacturing, transportation and distribution, use/re-use/maintenance, recycling, and final disposal (Boustead, 1993; Jimenez-Beltran, 1997). Three types of LCA are generally used for process or product development: cradle-to-grave, cradle-to-gate and gate-to-gate LCA. Cradle-to-grave LCA is usually used for product development. It defines the system boundary from materials extraction to disposal. Cradle-to-gate and gate-to-gate LCA are generally used for process development. Cradle-to-gate takes account of all the environmental burdens starting from materials extraction until the final production, while gate-to-gate LCA only accounts the burdens within the plant boundary i.e. from plant input gate to delivery gate.

LCA have two main objectives, the first is to quantify and evaluate the environmental performance of a process from 'cradle to grave' and thus to help the decision makers choose between alternative processing routes. In this context, LCA provides a useful tool for identifying the best practicable environmental option (BEPO). Another objective of LCA is to help identify options for improving the environmental performance of a process system (Cowell, 1999). In this way LCA can be employed as a stand-alone tool or combined with other P2 opportunity assessment tools for identifying the P2 opportunities over a broader environmental domain (Clift & Longley, 1995). Significant effort has been devoted to develop LCA databases and commercial tools for making the LCA more acceptable and easily applicable. Some common tools are 'Sima Pro', 'TRACI', 'Eco-it', 'Eco-Scan', 'TEAM™', 'CMLCA' etc., while common databases are 'IVAM LCA', 'The ecoinvent centre', 'Life cycle inventory database' 'GEMIS', 'CORINAIR', etc. However, LCA still suffers with some drawbacks, which need to be addressed (Weidema, 2000).

i) LCA is a highly data-intensive method, and the success of any given study depends on the availability of precise data, which is still an issue in LCA (Nourai et al., 2001).

ii) LCA system is still very time consuming and expensive; time and effort is wasted to duplicate the work already done by others (Bretz, 1998).

iii) Life cycle inventory (LCI) data are not still available for many industries in particular for chemical process units (Bretz, 1998).

iv) In LCA method serious difficulty arises during the evaluation phase, i.e. when effect scores of different impact categories are weighed against each other (Goedkoop and Spriensma, 2001).

v) LCA does not tell the investigator what is the ultimate limit of the environmental performance that can be achieved and thus it cannot help in proposing a specific corrective measure for attaining the target (Nourai et al., 2001).

vi) Significant uncertainties exist in LCA studies, which are very likely to introduce complexity in decision-making (Hulijbregts, 2000; Ragas, 1999; Bretz, 1998).

4.0 Overall Limitations of the Existing Frameworks

To-date, significant progress has been noticed in the direction of pollution prevention, nevertheless, it is far from complete. A significant number of limitations do exist which are listed below.

i) Lack of the adequate P2 identification phase (EPA, 1998; EPA, 1992)

ii) Lack of the adequate feasibility analysis phase (EPA, 1988; EPA, 1992)

iii) Lack of the consideration of other environmental management options (Figure 3.9) during P2 option selection. Due to the continuous improvement of technology, a recycling or end-of-pipe control approach may become more feasible technique than the selected pollution prevention option. There is a need to confirm that the selected P2 option is the optimum amongst the available environmental management options, otherwise sub-optimal P2 option may be selected, which would cause unsustainable solution.

iv) Lack of the consideration of risk and safety criteria during the feasibility analysis of different P2 options. Risk and safety assessment of P2 options is very important to reduce the potential damage to human health and ecosystems.

In this perspective, the present work is aimed to develop a systematic pollution prevention framework 'IP2M' (Figure 3.10) by addressing the above limitations, which is described below.

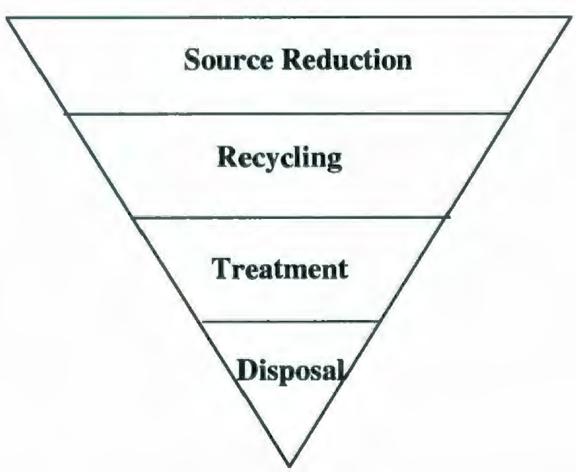

Figure 3.9: Hierarchy of Environmental Management Options (US EPA, 1992)

5.0 Details of IP2M Framework

5.1 Brief Description of Each Element of IP2M

5.1.1 Establishment of P2 Program

Top management support is very crucial to get a pollution prevention program started or to incorporate it into already existing activities and make the P2 as an organizational goal. Top management support can be achieved by outlining the advantages of P2. They should be informed that apart from the regulatory compliance, ecological and workers health and safety benefits, successful execution of the P2 program would benefit business in numerous ways, which include:

i) Cost savings through materials and energy conservation
ii) Increased productivity
iii) Improved product quality
iv) Reduction of potential long term liabilities
v) Reduced waste treatment, handling and disposal cost
vi) Improved public and corporate image

Once the management of all levels recognizes the value of adoption of P2, a policy statement should follow and be communicated to all employees. The next important step is to motivate all the employees to commit to successful implementation of the

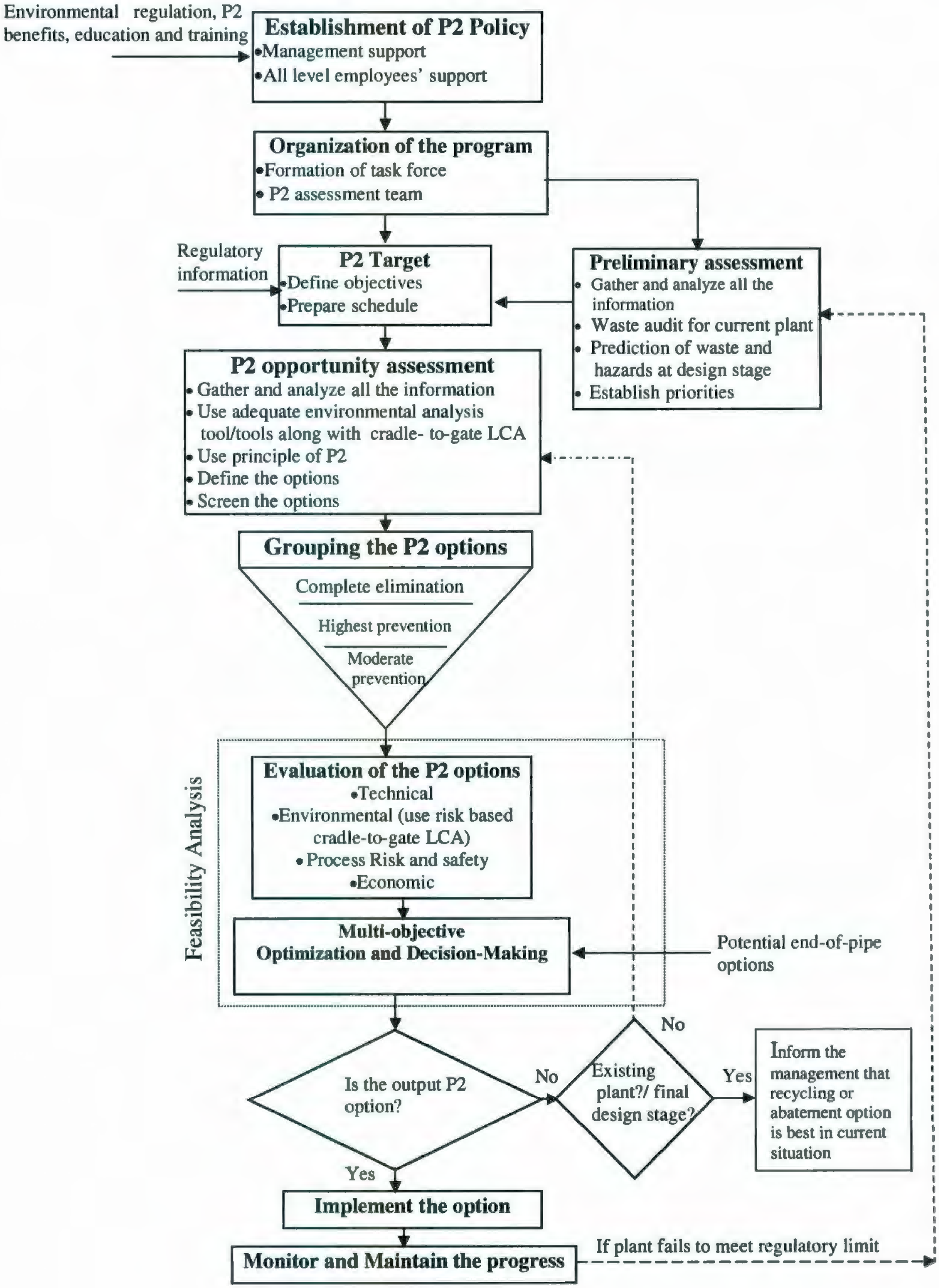

Figure 3.10: Proposed Pollution Prevention Framework (IP2M)

P2 program. The management should provide adequate trainings to all employees regarding the benefits of P2 so that they take P2 program as their own interest.

5.1.2 Organization of the Program

The step includes the formation of P2 task force and P2 assessment team. The task force should consist of representatives from all sections of the company, including administration, operations, technical evaluation team, maintenance, quality control, inventory, purchasing, finance etc. It should also include workers' representative from different sections, which would help to bring all the workers in the P2 program. The P2 task force will have the following responsibilities:

i) Setting pollution prevention objectives and time schedule
ii) Providing employees training and incentive program
iii) Oversee the program through its assessment, evaluation and implementation stages
iv) Overall evaluation of the P2 opportunity, selection and monitoring the progress
v) Maintaining the P2 program

The pollution prevention assessment team should consist of members having comprehensive knowledge in process, process machinery, process safety, environment, materials, process operations, maintenance and good computational, and analyzing capabilities. The pollution prevention assessment team with the help of the task force will identify the P2 options, group the options, evaluate and select the best option for implementation.

5.1.3 Preliminary Assessment

The purpose of the preliminary assessment is to identify the potential areas for detailed P2 study. In this phase, one important component is to gather and analyze the background information from the facility. It needs the proper understanding of processes involved and the wastes generated. The information include the type and quantity of raw materials used, the type and quantity of wastes generated, the individual production mechanisms, interrelationships between the unit processes and the cost involvement in production, utilities, waste treatment, waste handling, and disposal. For the existing plant, the amount of waste generated can be obtained from the waste audit, while for the plant at design stage, it could only be estimated via process modeling. Once all the background information has been collected, before conducting a detailed assessment, wastes and unit processes should be prioritized to determine which should be examined first. Establishing the priorities of streams are based on their toxic behaviors, quantity of waste, treatment, and other related costs.

5.1.4 P2 Target

P2 targets depend on the background information collected in the preliminary assessment phase and the regulatory level of a particular pollutant. It has two major elements: defining objectives and preparation of schedule. Objectives need to be stated in quantitative terms. After defining the objectives the assessment team needs to set a time schedule for different stages in order to achieve the targets. The time schedule considers the potential obstacles that might have to be encountered.

5.1.5 P2 Opportunity Assessment

Once the P2 target is defined, an in-depth study is needed to look into the unit operations associated with the target streams and then expanding the assessment throughout the entire facility to find out all the possible P2 options. A critical review and analysis of the detailed information on process, raw materials, equipments and costs help significantly to identify different P2 opportunities. The following information needs to be considered in the four different areas.

Process information

Process flow diagram

Flow through actual process

Process parameters

Correlation among different process parameters

Energy use

Materials Information

Physical and chemical properties of raw materials

Toxicity of materials and regulatory limit

Product composition and batch sheet

Product and raw materials inventory record

Life cycle toxicity and energy use and wastes information related to raw materials

Equipment Information

Equipment specifications

Performance data

Energy use

Accounting Information

Waste treatment, handling and disposal cost

Water and sewage cost

Cost for non hazardous waste disposal

Product, energy and raw materials cost

Operating and maintenance cost

The study also needs to be carried out in the area of supplemental operations such as utilities, maintenance, and house keeping. During the P2 opportunity analysis the principles of pollution prevention, which include mainly raw materials substitution, process redesign or modification, equipment addition/replacement, improved housekeeping, maintenance etc., need to be kept in mind. For P2 opportunity analysis numerous tools are available, which include mass integration and energy integration tools, graphical mass balance method, process simulation, life cycle assessment, etc. Except LCA tool, virtually all the available tools help to identify the P2 opportunities in the narrow system boundary by analyzing and optimizing process flow sheet or operating and design parameters of units. While, LCA integrates global environmental issues during process or raw materials selection and identifies the P2 opportunities over a broader domain. However, it does not have capability to analyze the process design or optimize the process parameters. In this context, an integration of LCA with other P2 opportunity analysis tools is crucial. In IP2M, it is suggested to use the cradle-to-gate LCA tool, a process simulation tool Aspen-HYSYS, a mass integration, and a heat integration tool in integrated manner.

After defining different P2 opportunities, screening is essential to sort out less costly and risk free options for immediate implementation. The other options need to go through detailed feasibility analysis phase prior to the implementation.

5.1.6 Grouping the Options

The available options need to be grouped in order to help to organize the evaluation procedure. The options need to be grouped based on principle of hierarchy – complete pollution elimination, highest pollution prevention, and then moderate pollution prevention. A group of P2 options are identified in this step that need to be evaluated in the next phase before implementation. If each option is evaluated separately before grouping, then after evaluation decision of grouping would be difficult as in separate evaluation the interactions between two options cannot be identified and grouping may produce different results than that anticipated from the separate evaluations. In this way, prior grouping can also significantly reduce the evaluation time.

5.1.7 Evaluation of the Options

In this phase, different grouped options are evaluated based on different objective functions. In existing P2 approaches, the P2 alternatives are evaluated based on technical, environmental and economic considerations only. In today's industries, risk and safety issues are recognized as important parameters due to the increased number of accidents. In order to reduce the potential impact to human health and ecosystems, a risk and safety assessment is an essential component of process evaluation. Therefore, in this approach, risk and safety is considered as an additional objective function to insure that the selected P2 option is within the acceptable safety limit. Technical evaluations examine ease of installation, maintenance, and operation. It also examines the extent of future modification and its degree of simplicity. An environmental evaluation compares the relative pros and cons of each P2 alternative with regard to their effects on environment. It investigates the impacts of a process option on human health and ecosystems. It also considers different global issues such as global warming, acid rain, ozone layer depletion, photochemical smog formation, etc., which have direct or indirect impacts on human health and ecosystems. It is challenging to determine the environmental consequences of weighing factors, which depend on several factors such as social context, industry location, and nature of the exposed population, country's overall pollution statistics, and likelihood of environmental occurrences. The success of pollution prevention initiative greatly depends on the robustness of the adopted environmental assessment tool. Therefore, in IP2M risk based cradle-to-gate life cycle assessment tool is incorporated for the environmental evaluation of P2 options.

Risk and safety assessment is concerned with the reliability of the process systems. It examines the options and determines the probability of any adverse impacts with respect to each option and the magnitude of such impacts. The economic evaluation estimates the total costs and benefits expected from the each group of options including cost savings and payback period.

5.1.8 Multi-objective Optimization

When the P2 options have been evaluated in terms of different objective functions then optimization should be carried out in order to select the optimum P2 option. In IP2M, the multi-criteria optimization and decision-making module simultaneously considers different P2 alternatives along with the potential end-of-pipe options in terms of different objective functions. This results in the P2 option, only when it becomes the most feasible environmental management option, otherwise the feasible end-of-pipe option will be selected.

For decision-making, in most of the existing P2 approaches priority based feasibility checking technique is adopted. In this approach, if an option is not feasible with respect to the first priority objective function then it does not proceed further. This does not always translate into the selection of the best option. In IP2M, optimization is suggested to carry out without considering the constraints. If the optimum P2/end-pipe-option exceeds any of the constraints in terms of any objective functions, then the optimized option needs to be reviewed in order to find out the possible improvements to satisfy the constraint. When the improvement is not possible, then the next prioritized option should be selected. The proposed optimization approach will allow the assessor to look at and think over the overall beneficial option and the possible direction of the improvements.

The evaluation of each P2 option in terms of any objective functions *k*, will give a single score $S_{s,k}$. In the proposed optimization approach, the score obtained for each objective function is to be multiplied by a weighting factor *w* to obtain a weighted score $W_{s,k}$. By adding the weighted scores for all the objective functions, the overall score, $S_{overall}$ of a P2 option will be obtained.

$$S_{overall} = \sum_{K=1}^{n} W_{s,k} \tag{3.1}$$

Where, n is the number of objective function. $S_{overall}$ will be the basis for selecting the best P2 /end-of-pipe option. Assigning of weighting factors and the value of different constraints depend on the company's policy based on the current situations. P2 task force together with the consent of top-level management decides those values.

5.1.9 Selection of the Option

Option selection is the most important phase. It depends on company's current standing. If the plant is at initial design stage, the best P2 option obtained in the multi-criteria optimization phase should be implemented. However, while at this stage the P2 option becomes unfeasible compared to the available end-of-pipe option, all the steps from P2 opportunity assessment needs to be thoroughly reviewed again for identifying the feasible P2 option (Figure 3.10). This is important because at initial design stage usually greater P2 opportunities exist. However, in case of existing plant or plant at final design stage, when the possible P2 options have already been incorporated, then further P2 options are not likely to be technically or economically feasible compared to the available end-of-pipe options. Therefore, at this stage if the P2 options become unfeasible, then the end-of-pipe option selected in the multi-criteria optimization phase should be implemented. In this way the proposed P2 approach can also serve as an environmental management tool.

5.1.10 Implement the Option

Once the P2 option is selected, the top management needs to be updated with a detailed report describing its technical, environmental, safety, and economic aspects. The report needs to clearly state the total implementation cost and anticipated return on investment with payback period. The report would help the management in taking the decision for its implementation.

5.1.11 Monitoring and Maintaining the Progress

Progress monitoring is important in order to get guidelines for future modifications. It embodies the quantitative measurement of reduction of the volume of waste and toxicity level as compared to the baseline value. Besides, the P2 project needs to be evaluated for its cost effectiveness, which could be done by determining either the payback period or net present value or return on investment. After implementation of the P2 option, if the emission level is observed to be higher than the current regulatory level or at any instant in future, due to the change of the regulatory requirements, if the plant fails to comply with the regulatory requirements, the P2 program needs to be thoroughly reviewed from the preliminary assessment phase. This step is essential in identifying and implementing the feasible P2 option to comply with the current or future regulatory requirements.

5.2 Features of IP2M

The different features of IP2M are discussed below.

a) It encompasses all the essential components of the P2 very systematically.

b) It proposes two-steps assessment. The preliminary assessment is useful for setting up the P2 objectives focusing all areas of concern, while the later step is concerned with the identification of the P2 opportunities subject to the set objectives.

c) It has added a phase 'grouping the options' based on the principle of hierarchy. This phase is important for organizing the options for evaluation.

d) It integrates a cradle-to-gate LCA tool, a process simulation tool (Aspen-HYSYS), a mass integration tool, and a heat integration tool in the P2 opportunity assessment phase. The LCA tool will allow for the identification of P2 opportunities over a broader environmental domain and the process simulation tool combined with the mass integration and heat integration tools will help take strategic decision for flow sheet modifications, equipment sizing and operating parameter changes. Use of these tools in the P2 opportunity assessment phase will allow the assessor for identifying the P2 opportunities extensively.

e) The evaluation of P2 options is based on multi-objectives. In this phase, IP2M has added one important objective, risk and safety, which examines the reliability of the process systems and predicts the probability of an accident to occur. In this way, it insures that the selected P2 option is safe for workers.

f) As the success of the P2 program greatly depends on the robustness of the environmental evaluation approach, in IP2M, for the environmental evaluation of the P2 options, risk based cradle-to-gate LCA tool is incorporated.

g) In multi-criteria optimization phase, IP2M simultaneously considers different P2 options with the potential end-of-pipe options in terms of different objective functions, which insures to select the optimum management option.

h) At the initial design stage of the facility, IP2M encourages to adopt the P2 option rather than using any end-of-pipe options. However, at this stage if the P2 options are not feasible it suggests reassessing the process systems thoroughly to identify the feasible P2 option. At final design stage, IP2M suggests the implementation of the end-of-pipe option if it appears better compared to the P2 options.

5.3 Applicability of IP2M

A qualitative study has been carried out to illustrate the applicability of IP2M briefly. The research is ongoing to demonstrate the applicability of different blocks of the framework quantitatively. The present case study considers the P2 program in an existing plant for the production of viscose staple fibre. This case study has earlier been used by Khan et al., (2002) to demonstrate the applicability of their proposed environmental management framework. The process is briefly described below.

Rayon grade pulp is steeped in a caustic soda solution and the excess lye is separated in slurry process to obtain a mat of alkali cellulose. After shredding, the alkali cellulose is reacted with carbon disulphide to yield cellulose xanthate. The xanthate so formed is dissolved in dilute caustic soda to give viscose, which is filtered, deaerated and ripened before extrusion through spinnerets into a spinning bath containing sulfuric acid, sodium sulfate and special additives. Cellulose is regenerated in the form of fine filaments. These filaments are cut into the required staple lengths, washed with disulphide, bleached and soft finished product dried to obtain viscose staple fibre, which is then baled in bailing press. Part of the carbon disulphide is recovered for reuse. The composition of the spinning bath is maintained by continuous removal of sodium and sulfuric acid.

5.3.1 Establishment and Organization of P2 Program

Top management should decide for undertaking pollution prevention program in their plant. This decision should be conveyed as a policy statement to all workers and staff and take adequate initiatives to train and motivate the workers. P2 task force is to be formed which will comprise the representatives from all the sections including workers. The P2 assessment team should be formed.

5.3.2 Preliminary Assessment and Target Setting

After characterizing the wastes and analyzing the waste removal cost the following P2 targets are identified:

- Reduction of Zn Emission

- Reduction of effluent discharge which are consist of four waste streams: i) lime water stream, ii) acid water stream, iii) alkaline stream, and iv) balance acid stream

5.3.3 P2 Opportunity Assessment and Options Grouping

The following P2 options can be identified in the viscose fibre plant by employing different engineering tools such as process simulation, mass integration, heat integration, and life cycle assessment tools.

- Use of the latest energy-efficient equipment such as multi-stage flash evaporators, continuous crystallizers and rotary compressors for stream and power conservation.
- Flow-sheet reconfiguration and optimization of operating parameters
- In-plant recovery
- Adequate maintenance and housekeeping

The maintenance and house keeping options could be screened for immediate implementation and the other options need to be grouped for detailed evaluation.

5.3.4 Evaluation and Multi-objective Optimization and Decision Making

The evaluation based on the technical, environmental, risk and safety and economic criteria are to be carried out for different P2 options. After the evaluations, the optimization needs to be performed based on the overall single score as mentioned in section 5.1.8 to select the best P2/end-of-pipe option.

5.3.5 Implementation and Progress Monitoring and Maintenance

The selected options are to be implemented and progress should be measured and if any of the target pollutants exceed the current regulatory limit or at any time in future the plant fails to comply with the changed regulatory requirements the P2 program needs to be reviewed.

6.0 Summary and Conclusions

The IP2M is designed for the systematic implementation of pollution prevention program during process design and retrofit applications. It is applicable for all types of process industries. It has been evolved with a significant number of features, which address the shortcomings of the previous frameworks developed in this area, and thus leads to a sustainable solution. The most important aspects of the framework are: i) it has integrated the cradle-to-gate LCA tool with other adequate P2 opportunity assessment tools such as mass integration, heat integration, process simulation tool etc., in P2 opportunity analysis phase, ii) it uses the risk-based cradle-to-gate LCA during the environmental evaluation of the options, iii) in evaluation phase, it has incorporated risk and safety as an additional objective function to insure that the selected P2 option is safe from occupational health and process safety aspect, and iv) finally the multi-criteria optimization and decision-making module simultaneously considers different P2 alternatives along with the potential end-of-pipe options in terms of different objective functions, which results in the P2 option, only when it becomes the most feasible environmental management option, otherwise the feasible end-of-pipe option will be selected.

These contributions in P2 evaluation and multi-criteria optimization phase help the analyst to select an environmental management option, which is overall beneficial concerning different objective functions including risk and safety. In addition, the integrated use of cradle-to-gate LCA tool along with other adequate P2 opportunity identification tools would make the P2 opportunity assessment more robust and help to find out the P2 options, which are friendly over the global environmental domain.

The effectiveness of the IP2M is not still authenticated by the quantitative case studies, however, the research is ongoing in that direction and the results will be reported soon.

7.0 Acknowledgements

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Chapter 4

Approach for Sustainable Process Systems Design (SusDesign)

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Preface

This manuscript chapter describes a process design approach by employing pollution prevention strategies at different levels of design, which has been submitted for publication in the *Journal of Applied Thermal Engineering*.

The work described in the manuscript is a result of the team group effort of the authors. The principal author (Khandoker Hossain) conducted literature search for concept development, identification and formulation of problems and developed the architecture of the approach. He was also involved in the case study design, execution, analysis and interpretation of the results and writing the first draft of the manuscript.

The co-authors (Drs. Khan and Hawboldt) supervised this work, and critically reviewed the developed approach. They also monitored the progress of the case study and reviewed the results and provided suggestions to revise the manuscript.

Abstract

This paper presents a structured process design approach, SusDesign, for the sustainable development of process systems. At each level of process design, design alternatives are generated using a number of thermodynamic tools and applying pollution prevention strategies followed by analysis, evaluation and screening processes for the selection of potential design options. The evaluation and optimization are carried out based on an integrated environmental and cost potential (IECP) index, which has been estimated with the IECP tool. The present paper also describes a flowsheet optimization technique developed using different thermodynamic tools such as exergy/energy analysis, heat and mass integration, and cogeneration/trigeneration in a systematic manner.

The proposed SusDesign approach has been successfully implemented in designing a 30 MW thermal power plant. In the case study, the IECP tool has been set up in Aspen HYSYS process simulator to carry out the analysis, evaluation and screening of design alternatives.

The application of this approach has developed an efficient, cost effective and environmentally friendly thermal system design with an overall thermal efficiency of 70% and CO_2 and NO_x emissions of 0.28 kg/kWh and 0.2 g/kWh respectively. The cost for per kWh of power generation is estimated as 4 cents. These achievements are significant compared to the conventional thermal power plant, which demonstrates the potential of the SusDesign approach for the sustainable development of process systems.

Keywords: Sustainable development, Process design, Exergy analysis, Cogeneration, Trigeneration, Optimization.

1.0 Introduction

In order to achieve sustainability, green as well economically viable process design is today's great challenge. In conventional process design, environmental issues are addressed by adopting the control technologies, which are not capable of achieving environmental as well as economic sustainability. Pollution prevention (P2) is receiving growing interest in process industries for sustainable process solution due to its considerable environmental and economic benefits. It is mainly achieved via reducing energy and mass usage in the process systems and the toxic release to the environment. Therefore, P2 can serve as a potential tool at different design stages for sustainable process systems design. The greater P2 opportunities exist in the preliminary design stage (Yang and Shi, 2000), when designers have sufficient flexibility to consider alternative designs.

A significant amount of work has been dedicated to incorporate environmental issues during the early stage of the process design (Azapagic et al., 2006; Dantus and High, 1996; Ciric and Jia, 1994; Crabtree and Elhalwagi, 1995; Gupta, and Manousiouthakis, 1994; Dunn et al., 1993; Richburg and Elhalwagi, 1995; Douglas, 1992). As a design objective, most of them have considered only cost, and environment is considered as a design constraint (Cano-Ruiz and McRae, 1998). Even in the recent process design books there are no clear guidelines as to how to incorporate environmental issues as design objective (Cano-Ruiz and McRae, 1998). In some studies, the environmental performance is only evaluated after complete flow sheet is developed and considered along with cost (Azapagic et al., 2006; Young and

Cabezas, 1999; Cabezas et al., 1999; Stefanis et al., 1995; Pistikopoulos et al., 1995). This cannot insure the design is optimum from an environmental viewpoint.

Douglas has introduced a hierarchical decision procedure for process synthesis and retrofitting to existing designs (Douglas, 1988). Subsequently the approach is modified for addressing waste minimization problem at the early design stages (Douglas, 1992). In this approach, the process synthesis activity is divided into five levels : i) input information, ii) input-output structure of the flowsheet, iii) recycle structure of the flowsheet, iv) specification of the separation system and v) energy integration. The approach provides systematic guidelines for hierarchical decomposition of flowsheet and screening of alternatives to quickly synthesize a number of potential candidate flowsheets. However, one major limitation is that due to its sequential nature, the interactions among different levels can not be accounted for (Beigler et al., 1997; Daichendt and Grossmann, 1997; Li and Kraslawski, 2004). Therefore, there is no guarantee that the developed flowsheet will be the optimum choice.

In the literature some other hierarchical approaches are also reported (Smith, 1995; Lewin, 2000; Alexander et al., 2000; Mexandre C. Dimian, 2003). At each level of synthesis, in the hierarchical approaches the cost is evaluated quantitatively, while, for environment a qualitative evaluation method is used. Unlike cost evaluation, quantitative environmental evaluation is not straightforward and prompt. There is a lack of a simple and quick quantitative environmental evaluation approach, especially for the evaluation of design alternatives during flowsheet synthesis.

Searching of design alternatives is mainly a knowledge based approach. Traditionally the effective use of knowledge greatly depends on the experience of the designers, which cannot guarantee in finding potential alternatives. Only a few design approaches have put some effort on how to use the knowledge based approach in an effective manner. In one approach, 'what if' questions are employed to generate some potential design alternatives for different elements of the process including raw materials, equipment, and procedures to improve efficiency, economic benefits, and reduce emissions (Jackson, 1997).

In a joint effort, Costain oil Co. and BP international developed ENVOP technique (Isalski, 1995) similar to the HAZOP, this technique uses a set of qualitative guidewords such as 'no', 'more', 'less' etc. to guide the designers for identifying some meaningful alternatives. There is still a lack of a systematic approach for effective use of the knowledge at different levels of flowsheet synthesis.

Over last few years, a significant amount of research has led to the development of several tools to systematically generate options to reduce either mass or energy usage or toxic emissions. Among these, some tools such as process simulation, mass integration, heat integration, energy and exergy analysis are demonstrated to be robust (Allen, 1997; Doerr, 1996; Elhalwagi, 1997; Linhoff et al., 1982; Azapagic, 1998; Rosen, 2008; Sengupta, 2007). In thermal process systems design, the implementation of exergy analysis, cogeneration and trigeneration facilitates the generation of energy efficient options (Rosen, 2008; Kanoglu, 2009; Mancarella, 2008; Sun, 2008).

The applicability of each of these tools to generate the potential design alternatives has been demonstrated separately in different applications. However, there is no such approach that integrates all these tools systematically in a design framework to guide the designers for generating design alternatives at different levels in preliminary process design.

In current design approaches, optimization of different alternative flowsheets is considered in the last step of flowsheet synthesis. For developing a few potential flowsheets, at each level of flowsheet synthesis, potential design alternatives are chosen based on subjective evaluation of economic, environmental and other criteria. This judgement depends on the experience of the designer and cannot insure the selection of the optimal options from a large number of options at each level of flowsheet synthesis.

In this context, the present paper proposes a systematic process design and synthesis (SusDesign) approach to address the limitations of the present methods. It has the following features:

i) Considers analysis, evaluation and screening of potential design alternatives at every level of the flowsheet synthesis.

ii) Integrates a set of tools at each level of synthesis to facilitate in searching, analysis, evaluation and selection of the potential alternatives.

iii) Employs an integrated environment and cost potential index (IECP) for evaluation, screening and optimization of alternatives (Hossain et al, 2009 or Chapter 5).

iv) Provides computational support for quantitative analysis, evaluation, screening and optimization of the design alternatives through the integration of IECP tool with a process simulator.

v) Incorporates the use of P2 guidewords and a few tools for effective use of knowledge during alternative search.

In this paper, the applicability of the SusDesign approach has been demonstrated through the preliminary design of a thermal power plant.

2.0 Description of the SusDesign Approach

The SusDesign approach is designed to provide a preliminary process design solution by incorporating environmental and economic issues from the initial stage of process design. Its main focus is to apply pollution prevention strategy via reducing energy and mass use and toxic emissions to achieve sustainable designs. The architecture of the SusDesign approach is shown in Figure 4.1. It divides the preliminary design of a process system into three major steps: i) process conceptualization, ii) flowsheet development and iii) flowsheet optimization. Each step goes through four sub-steps: i) alternative generation, ii) analysis, iii) evaluation and iv) screening. The SusDesign shows very systematically the different tools needed at each design phase. Three category of tools are used; the first category generates the design options, the second category is employed for analysis, and the third category is employed for evaluation and screening purposes. Most of the design analysis tools play dual roles, first, checking the way of alternative generation by analyzing the base option and second, assisting in performance evaluation of a particular design option.

2.1 Process Conceptualization Phase

This is the first phase for designing of any process systems and mainly concerned with the selection of process synthesis route. The proper selection of a process synthesis route is the major and critical decision part for the designers, as the economic, environmental, safety and other performances of a process system significantly relies on that selection. Once the process synthesis route is finalized, the scope of the improvement of process performance becomes narrowed down dramatically. The different steps in this phase are briefly discussed below.

2.1.1 Alternative Generation

The generation of design alternatives at this stage is mainly knowledge based. The designers should have in-depth knowledge of the process and applicability of different tools. The effectiveness of using a knowledge based approach greatly depends on the organization of knowledge. The use of some guidewords like 'no', 'less', 'more' etc. in HAZOP studies have been demonstrated to be effective for organizing knowledge of designers to find out the potential safety options during process design or retrofit activities (Kletz, 1983).

Pollution prevention is the main driving force in the proposed approach to generate environmentally friendly design alternatives. From the pollution prevention viewpoint, three guidewords i.e. 'elimination', 'minimization', and 'substitution' are used in the present approach to facilitate the organization of designers' knowledge to determine the potential alternatives with less design time. For the generation of alternatives, the first target should be elimination of the pollutants; where elimination is not possible, the designers may shift to minimization of the pollutants. If minimization is not able to reduce the toxicity and emissions to the desired level, then substitution of raw and ancillary materials and equipment could be considered. Pollution prevention consists of three strategies: source reduction, use/reuse and in-process recycling. In the proposed approach, the guidewords are applied to generate the alternatives relevant to the source reduction first, and then are used for the other

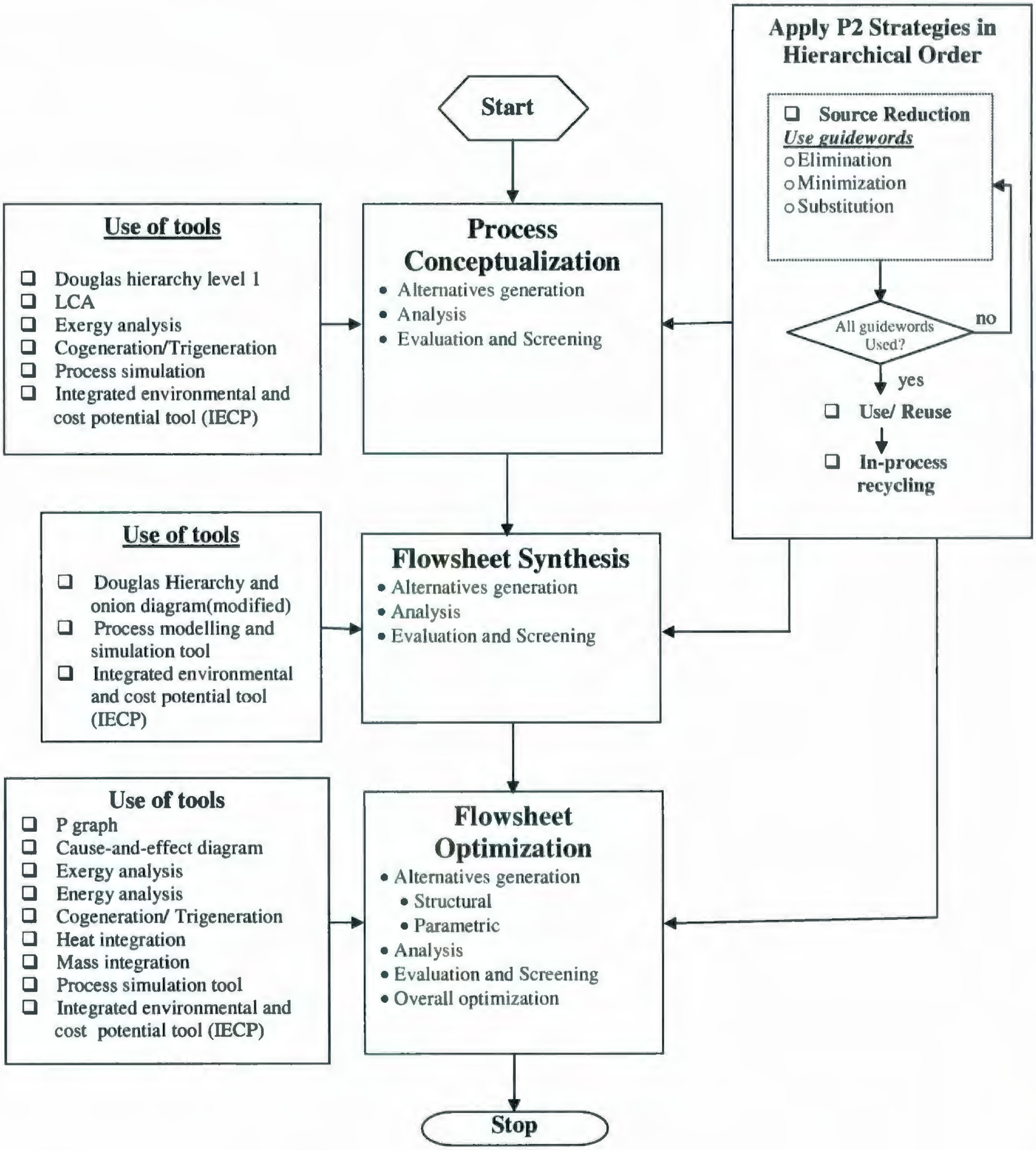


Figure 4.1: Framework for SusDesign Approach

two P2 strategies sequentially. In this way, the systematic use of guidewords in the P2 framework organizes the designers' knowledge for generating alternative design options.

In the proposed approach, four different tools are suggested to facilitate the generation of design alternatives in the process conceptualization phase: i) level 1 of Douglass hierarchy approach, ii) life cycle assessment (LCA), iii) exergy analysis, and iv) cogeneration/trigeneration.

The Douglas hierarchical decision procedure is used for selecting the design alternatives at different stages of flowsheet synthesis. The use of modified version of level 1 of Douglas hierarchical approach is proposed (Douglas, 1992). Level 1 is associated with the collection of nine categories of input information, which are specific to chemical process systems designs. Therefore, in order for level 1 of Douglas hierarchy to be applicable to all process systems, it is modified by adding four more information categories as shown in Table 4.1. The authors proposed the last four additional data categories to deal with a wide variety of process systems in addition to the chemical process systems, such as power generation systems, steel and cement manufacturing systems etc. All these information help the designers to think about the alternative options by employing P2 strategies.

At the conceptual stage, LCA can play an important role for identifying the materials of concern by assessing the materials over the cradle to grave system boundary. This provides the basis for the possible improvement of options concerning processing chemistry/technology, input or ancillary materials.

Table 4.1: Modified Level-1 of Douglas Hierarchy Approach

1.	Desired product, production rate, product value and product purity
2.	Reaction and reaction conditions
3.	Raw materials, streams, conditions and costs
4.	Data on the product distribution
5.	Data concerning the reaction rates and catalyst deactivation
6.	Any processing constraints
7.	Plant and site data and physical property data
8.	Data concerning the safety, toxicity and environmental impact of each of the
9.	Cost data for by-products produced
10.	Data concerning performance/efficiency of the process systems
11.	Exergy data in the exhaust streams
12	Available processing technology, necessary equipment and costs
13.	Cogeneration/trigeneration opportunities

Exergy is the maximum theoretical work obtainable from a system (Moran, 2004). The amount of work obtainable from a system depends on the surrounding conditions. The greater the difference between the system and its surrounding, the greater the work output from the system to surrounding (Ozturk et al., 2006). Exergy analysis can locate the processes/components important to be modified for improving the performance of a process or component through the evaluation of exergy destruction (Sengupta, 2007). Therefore, exergy analysis provides more realistic basis to the designers to identify the alternative options for improving the system's performance (Rosen, 2008).

Cogeneration refers to combined production of heat and power (CHP) in a power generation facility (Najjar, 2000). However, it could be applicable to any process system to exploit waste exergy. Trigeneration is the simultaneous production of cooling, heating and power, in one process facility (Khaliq, 2009). Like cogeneration trigeneration also could be applied to any process system. Through the use of waste exergy in another process within the same facility, cogeneration/trigeneration offers an energy efficient, environmentally and economically feasible process system (Kanoglu, 2009, Mancarella, 2008; Sun, 2008). At the conceptual stage, once the designers have the exergy analysis data of the base design, they can critically analyze the results to generate a few potential design alternatives by employing the cogeneration and trigeneration.

2.1.2 Analysis

Data analysis and generation of alternatives should be done simultaneously. Analysis of a base case data could quickly pinpoint improvement opportunities for generating potential design alternatives. The data should be analyzed from environmental, cost and safety perspectives. Analysis of alternatives also helps to readily screen out the inefficient alternatives and reduce the number of design alternatives for evaluation and further screening process. For analysis of design alternatives at conceptual phase the following tools are proposed to be used: i) life cycle assessment, ii) exergy analysis and iii) process simulation.

2.1.3 Evaluation and Screening

After the identification of the potential design options, it is crucial to evaluate and screen the options to choose the ones with the most potential. The SusDesign approach proposes quantitative evaluation based on the simultaneous consideration of environmental and economic criteria. To facilitate this, the present approach uses an integrated environmental and cost potential quantification (IECP) tool.

In IECP, the cost and environmental performance of a design option is evaluated in terms of cost and hazard index respectively. The cost index is estimated using Eco-index tool and for hazard index, Pro-hazard tool is used (Hossain et al., 2009). These two indexes are combined to have an IECP index, which is used as a basis for measuring the environmental and cost performance of an option compared to the base option. The IECP index could be calculated manually or using a process simulator by assigning an appropriate weighting factor to the cost and environment index.

If the value of IECP index of an option at this stage is considerably higher than other options then the option could be selected for further flowsheet design discarding others. However, if two or more options are reasonably close, then all of them should be selected for further flowsheet development.

2.2 Flowsheet Synthesis

Once the process synthesis route has been conceptualized and the process block diagram is defined, then the designers could proceed with the flowsheet synthesis, during this the following steps need to be followed:

2.2.1 Alternative Generation

Flowsheet synthesis have several stages, at each stage designers can generate potential design alternatives by using the modified Douglas hierarchy approach along with a process simulator.

The hierarchical design approach of flowsheet synthesis defined by Douglas has been demonstrated through some real life case studies (Rossiter et al., 1993). Smith (1995) has also proposed an onion diagram for synthesizing the flow sheet hierarchically. According to Smith, the synthesis should start from reactor, then separation and recycle, which are followed by heat exchanger network design, and finally utilities design. In the SusDesign approach the combination of Douglas hierarchy and Onion diagram is adopted with some modifications to make the approach applicable to all process systems. Table 4.2 lists the hierarchical steps proposed in flowsheet synthesis:

Table 4.2: Hierarchical Steps for flowsheet synthesis

i) Reactor/combustor design
ii) Feed material/energy stream preparation
iii) Flow sheeting the basic processes
iv) Recycle structure
v) Separation system design
vi) Feed preparation for separation system
vii) Design of cooling or heating systems

In the table three new steps have been added: step two, three and six. In step one, designers will search the alternatives in selecting particular reactor/combustor type, its design, and configuration. In some process systems such as thermal power generation systems, and steel manufacturing systems, a furnace/combustor is considered as a reactor. While for others such as hydro-electric systems, solar systems and wind turbine systems, where no reactor is involved, the designers will skip step one. The process system determines if a step is irrelevant.

By modeling a process, a process simulator helps to identify different alternative design options at each step of the flowsheet synthesis as shown in Table 4.2. During the flowsheet development, for generating the design alternatives at subsequent levels, the interaction effect with the previous levels needs to be considered, which is easily achieved when a process simulator is used.

2.2.2 Analysis: In the flowsheet development phase, the process simulator could be used to carry out the economic and environmental analysis of alternative options generated at each level of synthesis by examining the available data on equipment sizing, heat and power requirements, mass flow of raw materials and ancillary materials, consumption of utilities and mass separating agents, product and waste volume, and the emissions of toxic chemicals.

2.2.3 Evaluation and Screening

In the flowsheet synthesis phase, the IECP tool is set up in the process simulator to evaluate the alternatives at each level of flowsheet synthesis and screen out inefficient options. In this way, it gradually helps to develop potential flowsheet designs from environmental and economic viewpoint.

2.3 Flowsheet Optimization Phase

At this stage of the process synthesis, the flowsheet developed in the flowsheet synthesis stage is modified further to make it more sustainable. This phase also involves the basic steps such as alternatives generation, analysis, evaluation and screening. In addition, overall optimization is carried out at the end.

In the alternative generation step, minor parametric or structural modifications are carried out for the optimization of each individual flowsheet. For performing this, the flowsheet is examined rigorously by using a number of tools like exergy analysis, cogeneration/trigeneration, mass integration, heat integration etc., either independently or in concert with other tools.

In order to assist the designers to carry out the optimization task in a simple and effective way, a detailed algorithm for flowsheet optimization is developed which is shown in Figure 4.2. Before starting the optimization task one needs to identify the pollutants of concern and the sources of the pollutants/waste generation within the process system through the development of a P-graph (Halim and Srinivasan, 2002). A cause-and-effect diagram graphically represents different major P2 options available to eliminate or minimize the emission of the pollutants of concern (Ishikawa, 1990).

Figures 4.1 and 4.2 show that at first structural optimization should be carried out then parametric optimization and finally overall optimization. For structural optimization exergy/energy analysis, cogeneration/trigeneration, heat and mass integration tools are used.

Heat integration targets the minimum use of hot or cold utility in a system through the optimum use of the waste hot and cold process streams and thereby improves the environmental and economic performances of the systems (El-Halwagi, 1997). It looks into all the hot or cold streams of the process system in order to achieve the following tasks: i) proper matching of the hot and cold streams, ii) selection of the optimum amount of heating and cooling load that could be removed or added by each utility stream, iii) selection of the appropriate heating and cooling utilities iv) configuration of the heat exchanger net works for optimal performance.

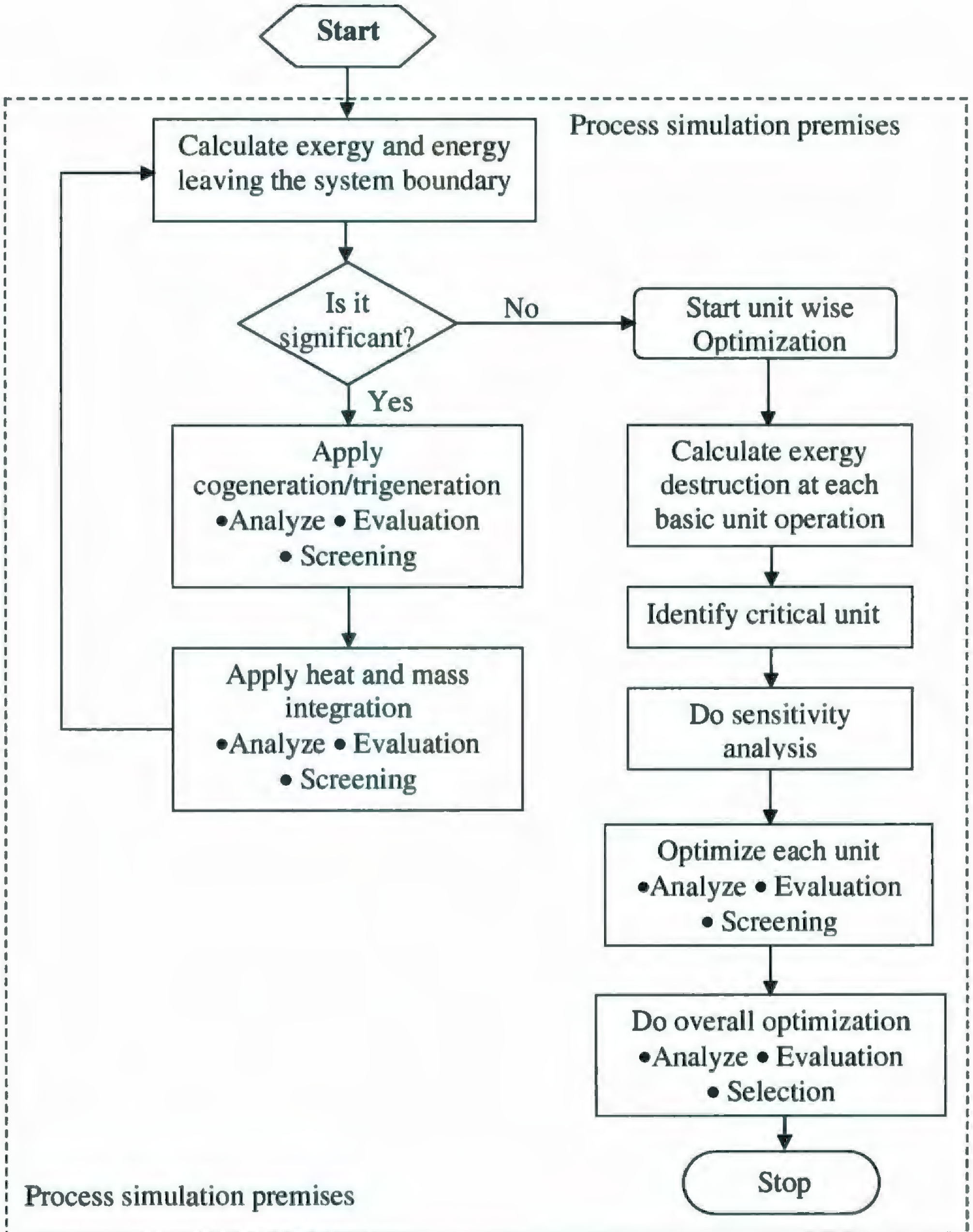


Figure 4.2: Detailed Algorithm of the Flowsheet Optimization

Mass integration is analogous to the heat integration. The main objective of the mass integration is to use the minimum amount of mass in the systems, especially the external mass separating agent. Therefore, effective use of mass integration reduces the operating cost and improves the environmental performance of the system. It considers various ways to achieve the desired goal such as manipulation of process equipment, structural changes in the flow sheet, selection of the mass separating agent, configuration of the separation systems rerouting of streams and addition of new units and so on (El-Halwagi, 1997; Noureldin and El-Halwagi, 2000).

For parametric optimization, exergy analysis is used in conjunction with a process simulator. This will generate a number of design alternatives which need to be analyzed and evaluated for selecting the potential alternatives.

During overall optimization each candidate flowsheet is optimized considering all the potential alternatives related to parametric change defined at different levels of flowsheet synthesis. The overall optimization will give an optimum flowsheet design considering the possible interaction effects among different unit operations.

The analysis of the design alternatives could be carried out by employing energy and exergy analysis, mass integration, heat integration and sensitivity analysis. For facilitating the analyses the process simulator provides energy and mass balance data of different design alternatives.

For the evaluation and screening of the generated alternatives related to optimization, the IECP tool also could be used. For screening out the inefficient alternatives during the optimization, the IECP index is set up as an objective function (to maximize) in the optimizer of Aspen HYSYS.

3.0 Application of SusDesign Approach

Case Study Description: For demonstrating the applicability of the proposed process design approach, a 30 MW thermal power plant design is considered. The target of the design is to achieve the sustainability. Throughout the design different alternative design options will be considered to minimize the cost and environmental impact as much as possible, while keeping the safety parameters within the boundary.

3.1 Process Conceptualization: Process conceptualization is the first phase of any design. At this stage the potential options will be generated and investigated with the aid of tools mentioned in the proposed approach. First, the modified Douglas hierarchy level 1 will be applied to collect the necessary information detailed below.

i) **Product specification:** The product is electric power of 30 MW. It will have continuous supply throughout the year.

ii) **Reaction Specification:** In a thermal power plant, fossil fuel reacts with the oxygen of the atmospheric air and generates heat and mixture of combustion products. The reaction occurs usually in gaseous phase. A set of kinetic reactions occurs depending on the choice of fuel and combustion parameters. In the case study, natural gas is considered as a fuel and for the combustion of the natural gas two steps kinetic reactions for CO and CO_2 formation are considered (Nieckeie et al., 2002) and a reduced one step kinetic reaction is considered for NO_x formation (Thompson et. al., 1972).

iii) **Raw materials/streams specifications:** For a thermal power plant design, at the conceptual stage, a range of raw materials are possible. For this case study coal, propane (LPG), and natural gas are considered as fuel. The average costs of natural gas, coal and LPG are about \$.25/m^3, \$0.036/ kg, and \$0.26/liter respectively (EIA, 2009).

iv) **Product distribution**: The product is only electric power which could be obtained due to the conversion of the rotational power of the steam or gas turbine shaft to the electric power via an electric generator.

v) **Reaction rates and catalysts deactivation**: The combustion efficiency for different fuels considered is high; therefore, catalyst is not important. However, in case of coal or crude oil combustion, depending on the amount of NO_x emissions, catalyst might be used to promote NO_x reduction reactions. In such case, catalysts poisoning occurs if fuel contains significant amount of sulfur.

vi) **Processing Constraints:** For safety, the design of any power plant should follow the maximum operating temperature and pressure limit for different unit operations. In general, in a gas turbine power plant, the operating temperature of any gas turbine should not exceed 1700 K (Moran and Shapiro, 2002) and the furnace should not run at positive pressure draft.

vii) **Plant Site Data**: A design site is considered which is 50 km far from the nearest population. The concentration of nitrogen oxides and sulfur dioxides in the centre of the populated area is considered as 0.02 ppm and 0.06 ppm averaged over a 24 hour period. The power transmission distance from the point of generation is taken as 70 km.

viii) **Safety/Toxicity/Environmental Impact Data:** Power plants generally emit CO_2, NOx, CO and unburned hydrocarbon. The amount of emission of a pollutant depends on the reactor design, fuel type, and combustion conditions. From the safety perspective most of thermal power plants are almost identical; however, the environmental impacts depend on the type of fuel.

ix) **Cost Data of byproducts:** For the base case, no byproduct is produced except power; however, using cogeneration/trigeneration cold or hot utility could be produced as byproducts. The cost of the cold and hot utilities could be calculated from the amount of electric power consumed to operate the systems to generate the utilities.

x) **Performance/Efficiency data:** The efficiency of a gas turbine thermal power plant ranges from 25-35%, while the efficiency for a steam turbine power plant is about 30-40%.

xi) **Exergy Data:** In a thermal power system, a significant amount of exergy is lost via the exhaust stream, which mainly depends on the processing technology. The exergy loss in a typical gas turbine plant through the exhaust gas is about 25% of the input exergy (Hashem, 1987), while in case of a typical steam turbine power plant it is about 1.7% (Gorji-bandpy and Ebrahimian, 2007).

xii) **Processing Technology/Equipment and Cost:** Two processing technologies are common in thermal power systems, Brayton cycle and modified Rankine cycle. The gas turbine power plant is based on the Brayton cycle; it is very compact and consists of compressor, furnace and gas turbine. The steam turbine plant is based on the Rankine cycle and is usually larger with more equipment. Otto/diesel cycle is usually used for small capacity power generation systems. They are very simple and compact. The startup procedure for a steam turbine plant is usually complicated and lengthy.

3.1.1 Alternatives Generation

After gathering all the information, the data is analyzed to create potential design alternatives by applying the P2 strategies and recommended tools. Application of these tools in context of the present case study is discussed below.

3.1.1.1 Source Reduction

The use of the elimination guideword for identifying P2 options could not be applied in the present case as the elimination of the emissions of CO_2, SO_2 and NO_x never can be completely achieved in a fossil fuel powered power plant. The minimization guideword is applied to generate some potential alternatives for minimizing CO_2, NO_x and SO_2 and unburned hydrocarbon emissions. One effective way of achieving such minimization is the use of cleaner fuel. For selecting the most potential fuel, three fuels such as coal, natural gas and LPG (100% propane) are studied. For defining the best fuel among the three options, the IECP index is determined by using the data on emissions, cost and toxicity for different fuels. For this comparison, basic gas turbine power plant is considered and coal is taken as the base fuel. The result of the assessment is shown in Figure 4.3.

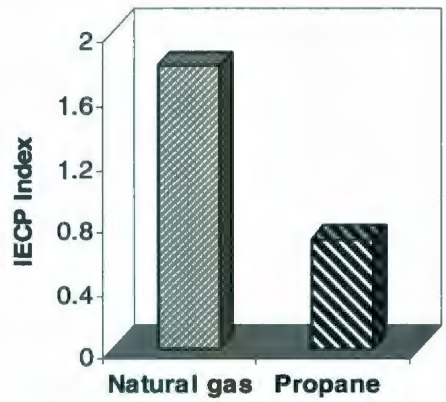


Figure 4.3: IECP Index for Different Fuels Compared to the Coal

The figure shows that natural gas has a higher IECP index compared to the propane. Both fuels have positive IECP index value, which indicates that both of them are better compared to coal. As natural gas has resulted in the highest performance, in present case study, natural gas is considered as the fuel for the proposed design. It is important to note that emissions of each fuel are quantified over the cradle to grave life cycle.

Another way to minimize the emissions is use of clean processing technology. By critically analyzing the information collected in section 3.1, it is obvious that two types of technologies could be considered for the case study i.e. gas turbine cycle power plant and steam turbine cycle power plant. For investigating which technology has more potential from both economic and environmental perspectives, exergy analysis is used.

3.1.1.2 Application of Exergy Analysis tool

The literature shows that the exergy loss with the exhaust gas in case of a gas turbine power plant is about 0.798 kW/kW of power output, while in case of a steam turbine power plant it is about 0.083 kW/kW of power output (Hashem, 1987). The efficiency of two types of plants are comparable (Polyzakis et al., 2008), however, since a large amount of exergy is wasted in the gas turbine plant, it has more potential for further improvement from economical and environmental perspectives.

3.1.1.3 Application of Cogeneration/ Trigeneration

The exergy analysis data shows a large amount of exergy is lost from a basic gas turbine plant via exhaust gas. The minimization guideword could be applied to reduce emissions from of the thermal system by reducing the waste exergy. The application of cogeneration/trigeneration could reduce the waste exergy significantly. In order to determine how they could be applied, one needs to examine the exergy data and temperature of the exhaust gas. In the present study, the investigation determines that the temperature of the exhaust stream is good enough to produce high pressure steam which could be used to drive a steam turbine power plant and in this way the waste exergy could be minimized. Therefore, it is decided to develop a cogeneration system by adding a steam turbine plant with the basic gas turbine power plant.

Literature indicates that the exhaust gas leaving a cogeneration plant still discharges some exergy and significant amount of heat (Hashem, 1987). Therefore, an extension of the system may be possible by employing the trigeneration through the installation of a vapor absorption refrigeration system or any process plant downstream that can use the waste heat. Based on the analyses carried out, a complete block diagram of the proposed thermal system sketched out which is used as the basis for the flowsheet development in the next design phase. The block diagram is shown in Figure 4.4. It is important to note that in present case study, the use of substitution guideword is not much related to find out the environmentally friendly design alternatives.

Other two P2 strategies i.e. reuse and in-process recycling are not applicable to the present case study at process conceptualization stage. It is important to note that depending on the case study, all P2 strategies might not be applicable to all design phases.

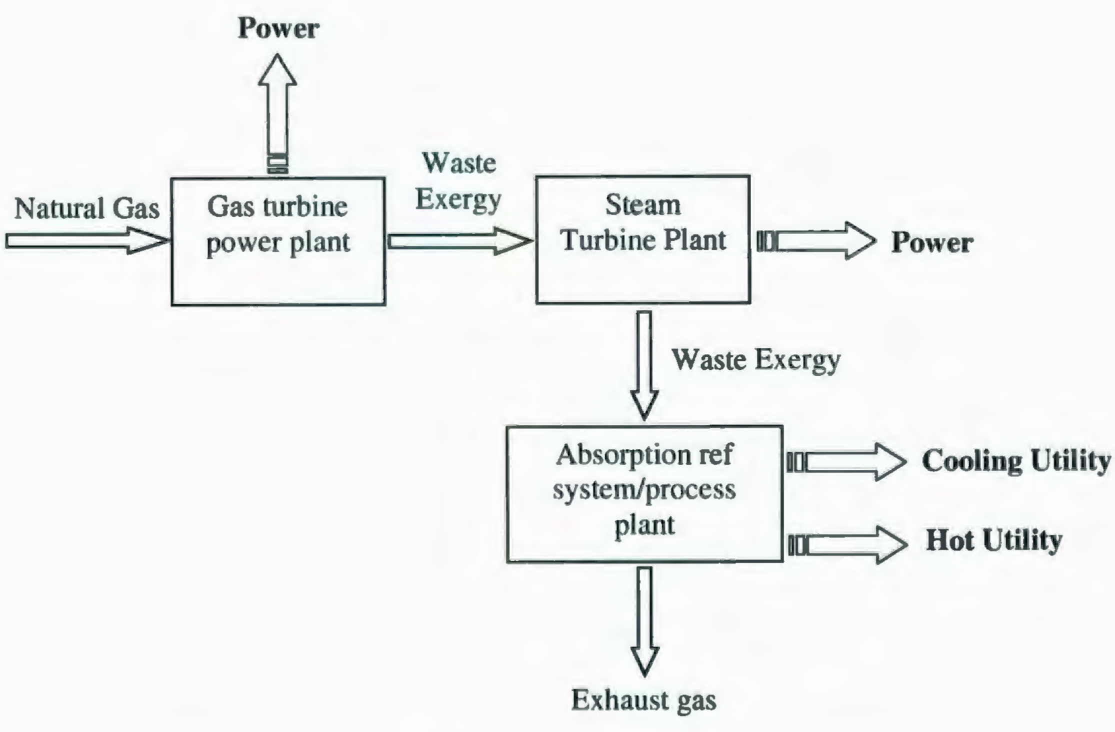


Figure 4.4: Block Diagram of the Proposed Power Plant Defined at the Process Conceptualization Phase

3.2 Flowsheet Synthesis

At this stage, based on the block diagram defined earlier, the flowsheet will be developed. According to the SusDesign approach, we will apply the use of modified Douglas hierarchy combined with onion diagram as shown in Table 4.2. Aspen HYSYS is used to model the process, which provides robust support to generate, analyze and evaluate design alternatives at each step of the synthesis.

3.2.1 Combustor/Reactor Design

After critically analyzing the reaction information collected in the conceptual stage, a plug flow type single combustor with circular cross section is selected. This is due to the fact that a plug flow reactor can better model the gaseous reactions occurred within the combustor. For selecting the size of the reactor it is important to investigate the effect of residence time on the emission of different pollutants. In order to carry out the study, a basic gas turbine power plant composed of three basic units is modeled using Aspen HYSYS process simulator shown in Figure 4.5.

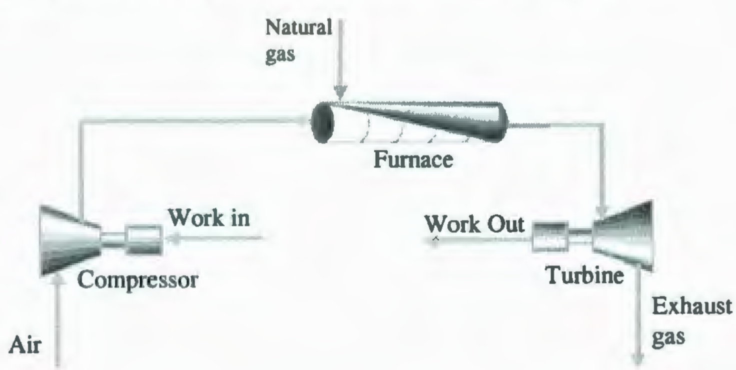


Figure 4.5: Schematic Diagram of Gas Turbine Cycle Power Plant

The effect of residence time on the emissions and power output is shown in Table 4.3 below.

Table 4.3: Effect of Residence Time on Plant Emissions.

Residence time sec	Mass flow of CO_2 kg/kWh	Mass Flow of NO_x mg/kWh	Mass flow of methane g/kWh
0.28	0.591	28.63	8.49
0.56	0.591	75.85	5.68
0.84	0.591	127.65	4.53
1.13	0.591	181.83	3.87
1.41	0.591	237.53	3.43
1.69	0.591	294.28	3.11
1.97	0.590	351.81	2.87
2.25	0.590	409.96	2.67

Table 4.3 shows that with the increase of the residence time the amount of unburned methane per unit kWh in the exhaust gas decreases. The emission of CO_2 per kWh decreases slightly, however, the amount of NO_x increases significantly due to the increase of the combustion temperature with the increasing residence time.

The analysis shows that the decision to select the optimal reactor size considering both the cost and environmental issues is not straight forward. Therefore, the IECP tool has been integrated with Aspen HYSYS to estimate the IECP index for different reactor options. The fixed cost, operating cost and the emission of pollutants of the plant were correlated with the residence time. The reactor having the residence time of 1.13 sec has been considered as the base case. As the simulation runs the IECP index for a residence time is calculated, the results are shown in Figure 4.6. The figure shows that the index values for the reactors having residence times below the base case are negative and above are positive. The higher the value is; the better the option is with respect to the base option. The negative values indicate that these reactor options are worse than the base option. The figure shows that that the highest value of the IECP occurs for the reactor with the residence time of 1.97 sec, therefore, for further development of the flow sheet this option is selected.

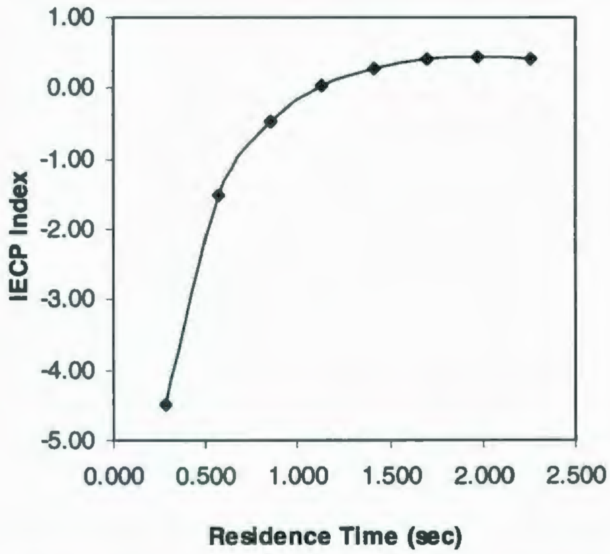


Figure 4.6: Integrated Environment and Cost Potential Index (IECP) for different residence time options

So, other potential reactor options will be considered during the overall optimization as this reactor option might not be ultimately selected when complete flowsheet is optimized considering all the possible interaction effects among different unit operations.

3.2.2 Feed Material/ Energy Stream Selection and Preparation

The main raw materials in the present study are fuel and air. In the conceptual stage, it is decided that natural gas is the best fuel option. At this stage, a few alternative options regarding the selection of the operating conditions of the raw materials such as air-fuel mixtures, inlet air temperature and compression ratio are studied. At first different options of air-fuel mixture are considered. The temperature of the combustion product, emissions, and net power output of the plant significantly varies with the air-fuel ratio.

For this study, the actual air-fuel ratio to stoichiometric air-fuel ratio (λ) is varied within the range of 1 to 2.5 for a constant compression ratio of 10. The option with λ of 1.5 is considered as the base option. The change of air-fuel ratio for a fixed amount of fuel impacts the size as well as the cost of different components. In this study, the amount of fuel has been fixed and the amount of air is varied to get different options of air-fuel mixture. For screening out the options with less potential, during the simulation IECP index has been calculated by Aspen HYSYS for each option which is shown in Figure 4.7.

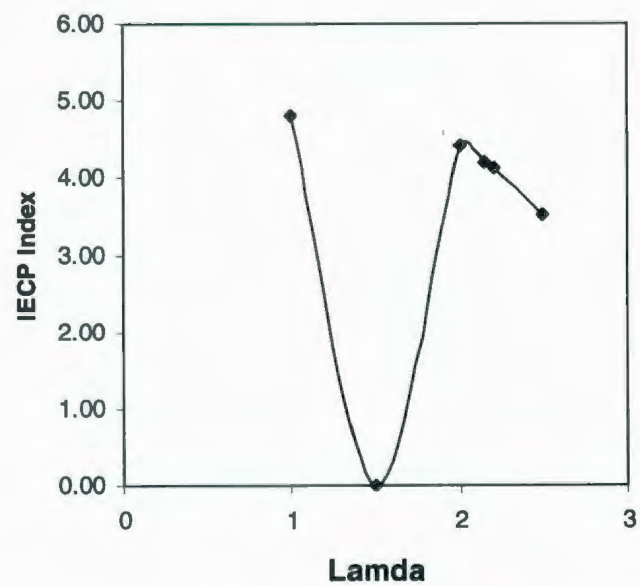


Figure 4.7: IECP Index for Different Values of λ.

The figure shows that the index value is the maximum at λ of 1, then the next maximum is observed at λ of 2, afterwards it decreases with the increasing value of λ. This indicates that all investigated options have better overall potential than the base option. Due to the limitation of the turbine material the temperature of the combustion product should not exceed 1700 K. Simulation studies show that at λ of 1 and 2, the combustion temperature exceeds the limit, therefore, among the available options the option with λ of 2.15 is selected due to its highest IECP index value.

Next different pressure options at the compressor outlet are investigated. Several pressure options have been considered within a range of 800 kPa to 1400 kPa. The base option is considered as 900 kPa. Figure 4.8 shows that as compressor exit pressure increases the IECP index increases. The emissions and combustion temperature data for different pressure options are shown in Table 4.4.

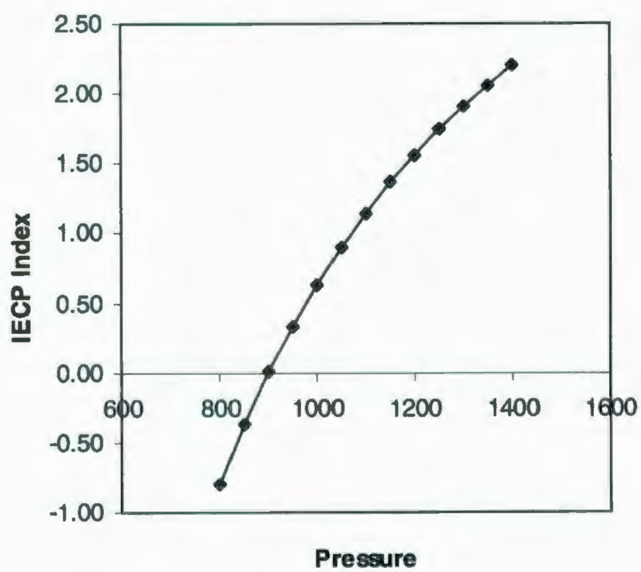


Figure 4.8: IECP Index for Different Compressor Exit Pressure Options

Table 4.4: Emissions and Power Output for Different Pressures at Compressor Exit.

Pressure [kPa]	800	900	1000	1100	1200	1300	1400
CO_2/kWh	0.67	0.65	0.62	0.61	0.59	0.58	0.57
NO_x g/kWh	0.05	0.09	0.14	0.21	0.30	0.42	0.58
CO g/kWh	0.15	0.10	0.07	0.05	0.04	0.03	0.02
Temperature [K]	1620	1636	1651	1664	1677	1689	1700
Net power output (MW)	14.84	15.42	15.92	16.35	16.73	17.07	17.37

The table shows that with the increasing pressure, the emissions of CO_2 and CO for a unit kWh power output decreases, however, the emissions of NO_x increases. This is due to the fact that as pressure increases the combustion temperature increases which causes higher NO_x emission. Although Figure 4.8 shows that the 1400 kPa pressure option shows highest potential, it produces high temperature combustion product at 1700 K. Therefore, for safety consideration the 1200 kPa pressure option is chosen.

In the next step, we will examine the effect of the inlet air temperature on the performance and emissions of the plant are studied. The air temperature is reduced from 25 °C to 8 °C at λ of 2.15 and 1200 kPa compressor exit pressure. The results are shown in Table 4.5, which shows that both the net power output and emission performance of the system improves gradually as inlet air temperature decreases.

Table 4.5: Effect of Inlet Air Temperature on Plant Emissions and Power Output

Air Temperature [°C]	25	22	18	15	10	8
Net work output [kW]	16510	16548	16598	16637	16700	16726
CO_2 kg/kWh	0.60	0.59	0.59	0.59	0.59	0.59
NO_x g/kWh	0.24	0.21	0.18	0.16	0.13	0.12
Methane g/kWh	0.04	0.04	0.05	0.05	0.05	0.05

Furthermore, the reduced inlet air temperature lowers the temperature of the combustion product, at 8 °C inlet air temperature, combustion product temperature reduces to 1366 °C from 1404°C. This provides a clear advantage to let the compressor pressure increase slightly to set the temperature to 1404°C in order to get improved power output and reduced emission/kWh. In this way, input temperature reduction can give twofold benefits to improve the performance of the plant.

To reduce the inlet air temperature from 25°C, the vapor compression refrigeration system has been considered. The addition of this system will certainly have some environmental and economic impact. Therefore, we investigate if inlet temperature options including vapor compression refrigeration system have potential and if so which option has the highest potential. The amount of major emissions to produce the unit amount of refrigerant R134 has also been considered. The investigations of different input temperature options have been carried out for a fixed combustion temperature at 1404°C by varying the compressor exit pressure.

Figure 4.9 shows that for all investigated inlet air temperature options have negative IECP index, indicating that the base option i.e. inlet air at 25°C without cooling is the best option. This is due to the fact that although increased amount of

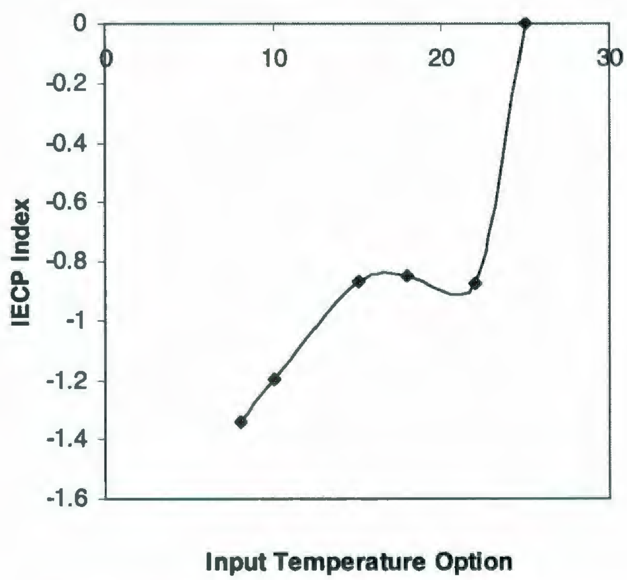


Figure 4.9: IECP Index of Different Input Air Cooling Options for Cooling the Inlet Air Temperature

cooling improves the net power output of the thermal system and keeps the emission performance almost unchanged, however, the per kW-year fixed cost of the system increases for the addition of the refrigeration plant. This makes all temperature cooling options less potential compared to the base option or non-cooling option. Therefore, based on this investigation it is decided that the temperature of the inlet air would be kept at ambient condition.

3.2.3 Flowsheeting the Basic Processes

The basic flowsheet is developed according to the defined block diagram as shown in Figure 4.4. For this development Aspen HYSYS process simulator is used. The schematic diagram of the basic flowsheet is shown in Figure 4.10.

The waste exergy from the gas turbine exit is exploited via the generation of high temperature and pressure steam in a heat recovery steam generator unit (HRSG). The flowrate of the steam is maintained so that the exhaust gas temperature from the HRSG remains about 100°C. The steam is passed over a steam turbine which gives some additional work output. As a result, the net work output of the cogeneration plant becomes about 28.5 MW compared to 16.5 MW obtained for a basic gas turbine plant. This gives the overall thermal efficiency of the cogeneration system as 57%. In this study, a simple steam turbine plant has been considered and this steam reheating is not considered in HRSG. The performance of a steam turbine plant greatly depends on the pressure and temperature of the steam. In order to investigate any possible interaction effect between temperature and pressure they are varied simultaneously. The result is shown in Table 4.6. The table does not show any interaction effect between temperature and pressure on the net work output. It shows that at higher temperatures and pressures the plant output becomes higher. At this point one needs to decide which temperature and pressure options have more potential from environmental and economic viewpoint.

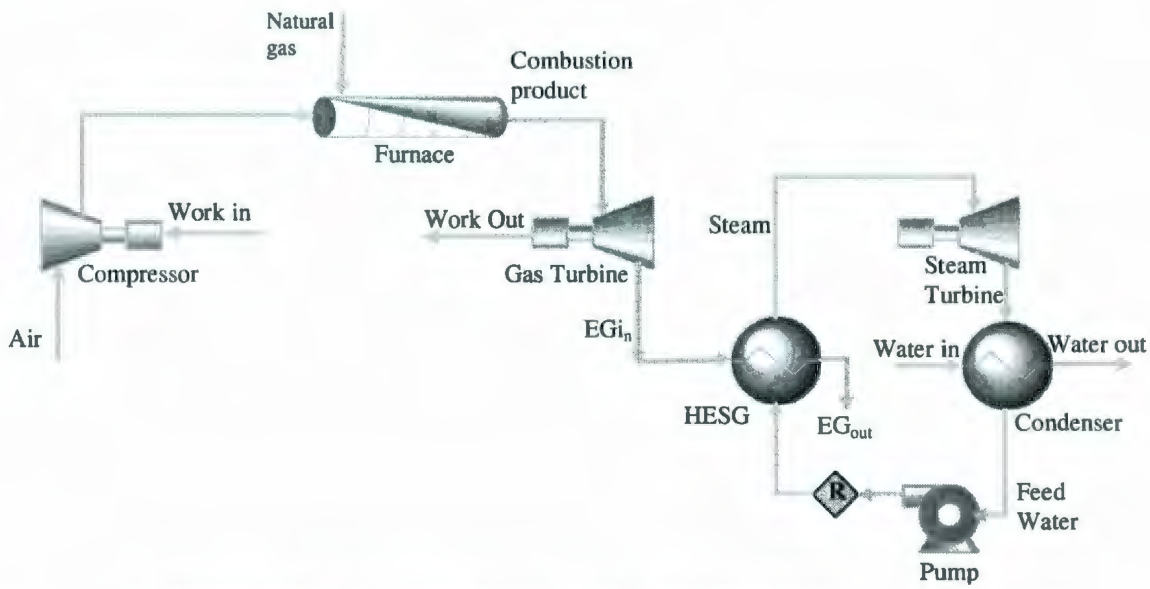


Figure 4.10: Schematic Diagram of the Thermal Power Plant Defined in the Conceptual Stage

Table 4.6: The Net Power Output of the Plant at Different Temperatures Pressures Combinations

Temperature, °C	Pressure, bar	Net Power out put MW
400	100	27.33
400	140	27.65
400	180	27.81
500	100	27.70
500	140	28.05
500	180	28.24
600	100	28.12
600	140	28.47
600	180	28.68

The investigations have been carried out for a pressure range of 80-200 bar and a temperature range of 350 to 650°C. The IECP index for each pressure and temperature option is calculated by Aspen HYSYS. The results are shown in Table 4. 7.

The results show that at higher pressure and temperature combinations the IECP index becomes higher and the highest value is obtained for the option having the maximum temperature and pressure. This is due to the fact that for increased temperature and pressure options the work output increases, which decreases the operating cost/kW-year and all the major emissions/kWh.

Table 4.7: Integrated Environment and Cost Potential and Emissions Data for Different Steam Temperature and Pressure Options.

Temperature, °C	Pressure, bar	IECP	CO_2 kg/kWh	NO_x g/kWh
350	80	-0.89	0.37	0.17
350	120	-0.49	0.36	0.17
350	160	-0.33	0.36	0.17
350	200	-1.83	0.38	0.18
425	800	-0.67	0.37	0.17
425	120	-0.25	0.36	0.17
425	160	-0.05	0.36	0.17
425	200	0.04	0.36	0.17
500	80	-0.40	0.36	0.17
500	120	0.00	0.36	0.17
500	160	0.21	0.35	0.16
500	200	0.34	0.35	0.16
575	80	-0.13	0.36	0.17
575	120	0.27	0.35	0.16
575	160	0.48	0.35	0.16
575	200	0.62	0.35	0.16
650	80	0.16	0.35	0.17
650	120	0.53	0.35	0.16
650	160	0.75	0.35	0.16
650	200	0.89	0.34	0.16

Although the fixed cost of the equipment/kW-year increases, the rise is less compared to the decrease in the operating cost. Further, benefits are added due to the decreased emissions. The cumulative effect results in the increased IECP. It seems that at further higher pressures and temperatures the net benefit will be higher; however, at this point the option with 200 bar pressure and 600°C temperature is considered, further study will be carried out at flowsheet optimization stage.

3.2.4 Recycle Structure

At this stage, the possible recycling opportunities are studied. As a recycling option, a portion of flue gas is recycled to cool down the furnace temperature for reducing the emission of NO_x. Table 4.8 shows the impact of different amount of flue gas recirculation on the plant power and emission performance.

Table 4.8: The Impact of Flue Gas Recirculation on Plant Emissions and Power Output

Recirculation (%)	Net Power [kW]	CO_2 [kg/h]	(NO_x) [kg/h]	Methane [kg/h]
0	28,311	9,952	4.64	0.66
5	28,162	9,951	1.74	0.93
10	27,993	9,950	0.62	1.34
15	27,798	9,948	0.20	1.96
20	27,579	9,946	0.06	2.92
25	27,324	9,942	0.02	4.42
30	27,026	9,935	0.00	6.75
35	26,666	9,926	0.00	10.24

The table shows that as flue gas recirculation increases the NO_x emission decreases significantly due to gradual cooling of the combustion gases. The results also show that emissions of carbon dioxide and unburned methane increase but net power output decreases significantly with the increasing recirculation. The net power output decreases for two distinct reasons: first, due to the additional energy requirement for flue gas delivery, and second, due to the increased amount of recirculation, the temperature at turbine exit decreases which results in the decreased steam temperature.

At this point, with the aid of the IECP index, different options of flue gas recirculation are studied. For this, the option without flue gas recirculation is considered as the base case. Figure 4.11 shows that for all investigated recirculation options, IECP index is negative and the situation becomes worse with increased amount of recirculation. The results indicate that the base option is the best among the investigated options. This is due to the fact that through the recirculation, although the NO_x reduction per kWh decreases, however, at the same time per kWh CO_2 emission, fixed and operating costs increase. Therefore, in this context, the flue gas recirculation is not selected.

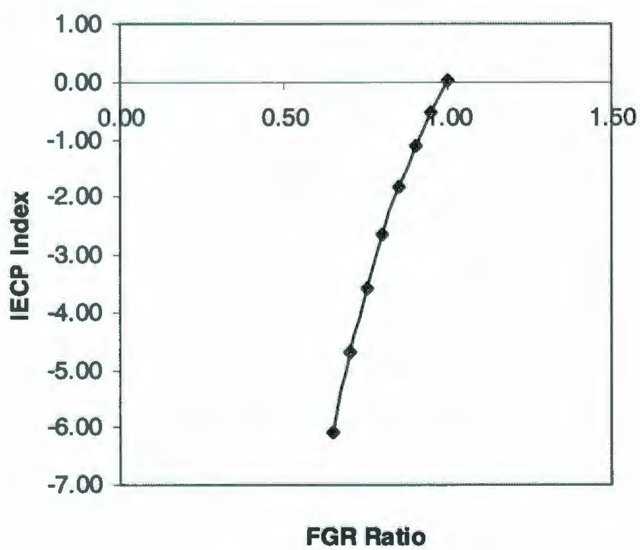


Figure 4.11: IECP Index for Different Flue Gas Recirculation Options.

Next we have considered the recycling of the condenser cooling water. In practice, in most cases condenser cooling water is recycled except where abundant water source is available near the plant. Water recycling option reduces pumping cost, water treatment cost and increases the life of the condenser. It reduces the pollution by reducing the energy use and water treatment chemicals. On the other hand, the recycling option involves the fixed capital cost for cooling tower. Taking all these into account IECP index for the recycling option is determined compared to the non-recycling option which is 0.2. Therefore, for the present case, water recycling option is chosen.

3.2.5 Design of Cooling or Heating Systems

For the present case study, separation system can not be used; therefore, we look into the last step of Table 4.2 which is related to the design of the cooling or heating system. Under this, we investigate the potential cooling options for condenser water cooling. Traditionally for cooling the condenser water, a cooling tower is used. In this study, a sieve type tray column is considered which is modeled by using Aspen HYSYS.

The results are compared with the data of the conventional cooling tower recycling system. The ambient air at 25°C having moisture content of 18.2g/kg of dry air is considered as the input of the column. The wet bulb temperature of the air is about 23.9°C. The column is initially modeled with 10 trays of 1.5 meter diameter, which might be changed due to flowsheet optimization. The water loss due to the cooling operation in column is calculated by Aspen HYSYS, which is about 23 ton/hour. In the column, the condenser water is cooled by evaporative cooling as cooling tower. However, as cooling tower design is open type, some additional water is lost due to windage loss. Besides, air-water mixing is better in the column due to its close type design and thus airflow requirement for a particular amount of cooling would be reduced, which would eventually reduce the operating cost of the blower. The value of the IECP index considering the cooling tower as a base option is calculated as 0.6, which indicates that the cooling in a sieve type tray column is the better option as compared to the conventional cooling tower option.

3.3 Flowsheet Optimization

In this phase, the flowsheet developed in the previous phase is further investigated to make it more sustainable. For the optimization of the flowsheet we have used our proposed algorithm shown in Figure 4.2. Prior to the optimization, a P-graph is developed to identify the pollutants of concern which is followed by a cause-and-effect diagram to identify the major ways needs to be adopted during the optimization process to reduce the environmental concerns.

3.3.1 P-Graph

In the present case study, the emissions from the stack are predicted by Aspen HYSYS. The emission of NO_x is 33 ppm, which is much lower than the regulatory limit. Unburned hydrocarbon and CO emissions are observed to be very low.

Therefore, key concern is related to the present study is CO_2 emission. To identify the source of CO_2 formation within the plant P-graph is drawn (Figure 4.12).

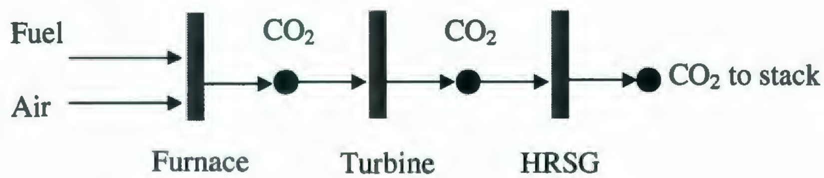


Figure 4.12: P-Graph for CO_2

The graph shows that the furnace is the only source of CO_2 generation. So, one can pay more attention to the combustion process in the furnace to reduce the CO_2 emission.

3.3.2 Cause-and-Effect Diagram

From P-graph it is identified that furnace is the only source for CO_2 generation, however, it does not provide any solution how to reduce CO_2 emission. The cause-and-effect diagram in Figure 4.13 shows that the emission of CO_2/kWh could be reduced through raw materials change or design modifications.

In this case study, as a raw material, natural gas is used which is composed of 100% methane. Of the fossil fuels, methane has the minimum C to hydrogen ratio. Therefore, in present case the option of changing the raw material is not open. The diagram shows that CO_2 generation/kWh could be reduced by implementing three design modification options: i) reducing energy use in different units, ii) increasing power output of the system and iii) reducing energy loss from the exhaust gases. All these could be achieved by parametric/structural modifications. For achieving these three major tasks, different tools are applied in following sections according to the proposed optimization algorithm as shown in Figure 4.2.

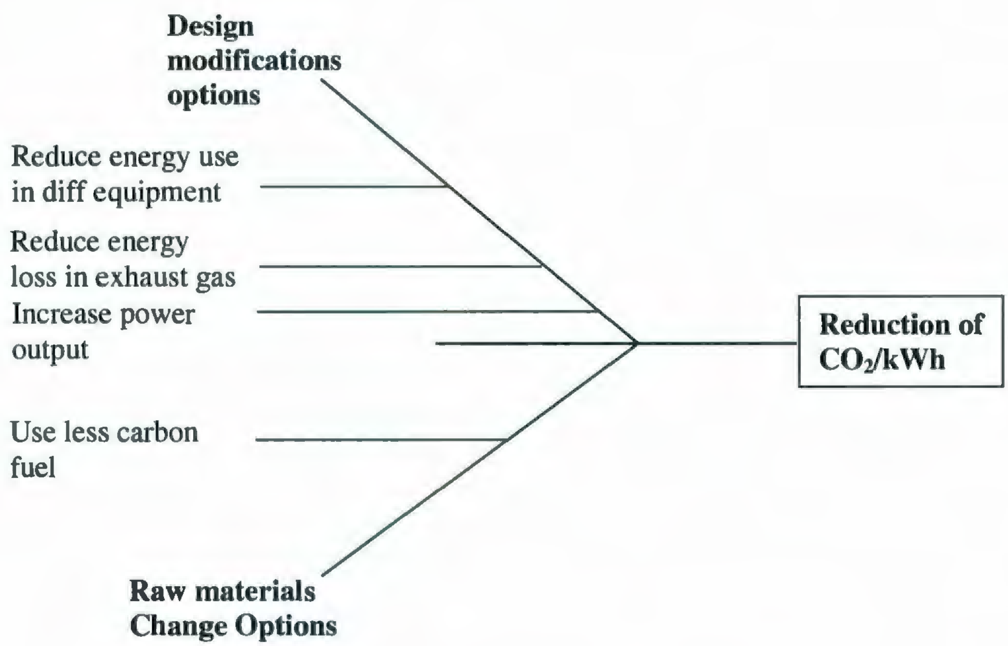


Figure 4.13: Cause-and-effect Diagram for CO_2 Reduction

3.3.3 Structural Optimization

For structural optimization several tools have been used in concert with Aspen HYSYS process simulator, they are described below.

3.3.3.1 Exergy/Energy Calculation

For structural optimization of the flowsheet according to the proposed optimization approach, exergy and energy calculation of all the streams leaving the system boundary is recommended. However, for parametric optimization, exergy destruction at every unit operation needs to be calculated. The required exergy and energy for different streams and exergy destruction for different unit operations are calculated with the aid of Aspen HYSYS which are given in Table 4.9. The isentropic efficiency for compressor, gas turbine and steam turbine is considered as 85% during their modeling in flowsheet synthesis stage.

Table 4.9: Calculation of Exergy for Different Streams and Exergy Destruction at Different Unit Operations.

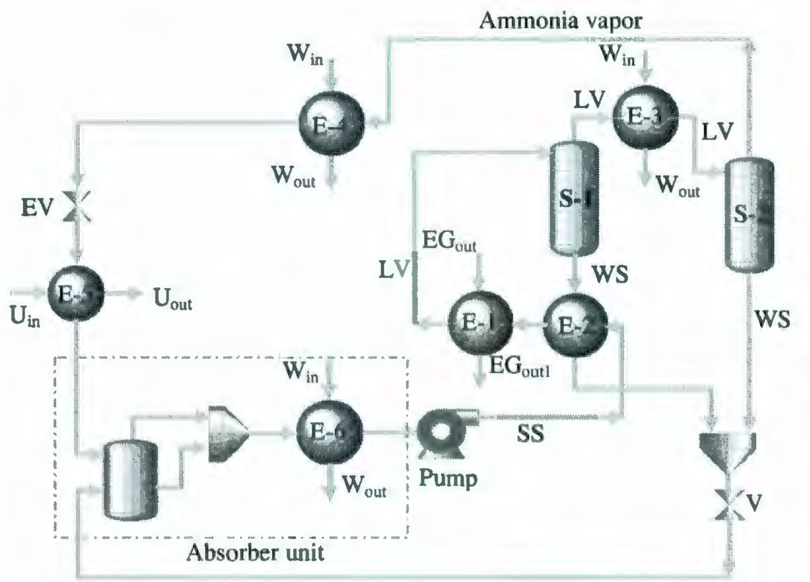
Unit operations	Streams	Energy value (MW)	Exergy Value (MW)	Exergy destruction (MW)	Exergy destruction (%)
Air comp		-	-	0.805	6.69
Furnace		-	-	15	23.706
Gas Turbine		-	-	1.567	4.96
Steam turbine		-	-	1.314	9.60
HRSG		-	-	2.45	14.74
HRSG	Exhaust gas	6.83	1.1	-	-
Feed pump		-	-	negligible	-
Condenser	Cooling water out	16.46	negligible	-	-

The exergy values have been calculated with respect to a reference temperature and pressure at 25°C and 101.325 kPa, while neglecting other potential and kinetic energy effects. For calculating the chemical exergy, model II (Szargut, 1988) is considered. The energy value is also calculated with respect to the same reference conditions and effects of kinetic energy and potential energy have been neglected. Two streams leave from the system: exhaust gas and condenser cooling water. Table 4.9 shows that the exergy wasted via the exhaust gas is 1.1 MW, while the energy value is 6.83 MW. As the exergy value is not significant, therefore the use of exhaust gas to have some useful work is not recommended. However, in the exhaust gas the energy value in form of heat is significant and as it has some exergy value as well, thus a major part of this heat could be effectively used to produce some heating service. The condenser cooling water is carrying a large amount of heat energy, but negligible exergy and is not useful. This analysis leads us to consider another system downstream to produce either some heat or cold utility which will make the overall system as a trigeneration system.

3.3.3.2 Application of Trigeneration

In order to recover the waste exergy as shown in Table 4.9 trigeneration concept is used to produce some cooling utility via an absorption refrigeration system to support or replace the conventional air-conditioning or refrigeration system operated by a vapor compression refrigeration cycle. Aspen HYSYS is used to model the absorption refrigeration system. As a refrigerant, ammonia-water solution is used. The exhaust gas at 100°C is used to heat the generator. The schematic diagram of the vapor absorption system is shown in Figure 4.14.

The major operating parameters and the coefficient of performance (COP) of the system are shown in Table 4.10 below. In the vapour absorption system underground water at 20°C is used as a cooling utility. Water is lifted from 200 ft below the ground surface. The diameter of the pipeline is considered as 0.25 m and the isentropic efficiency of the pump is considered as 85%.



E-1: Generator
E-2: Exchanger
E-3: Exchanger
E-4: Condenser
E:5: Evaporator
E-6: Exchanger
S1: Primary separator
S2: Secondary separator
V: Valve
EV: Expansion valve
LV: Liquid-vapor mixture
SS: Strong solution
WS: Weak Solution
W_{in} : water in
W_{out}: Water out
EG_{out}: Exhaust gas out From HRSG
EG_{outl}: Exhaust gas out from generator
U_{in}: Utility in
U_{out}: Utility out

Figure 4.14: Schematic Diagram of Vapor Absorption Refrigeration System

Table 10: Operating Parameters and Characteristics of the Vapor Absorption Refrigeration System

Absorption Pressure	477 kPa
Condensation Pressure	1220 kPa
Water/ammonia ratio	1.65
Condensation temperature	31.79°C
Exhaust gas temperature	100°C
COP of the system	0.515
Cooling effect produced	1012 kW
Utility required	125.9 ton/h
Power required	30.2 kW

In COP calculation, the power required for delivering the water and pumping the refrigerant have been considered. The table shows that the vapour absorption system is able to produce 1012 kW cooling effect. To produce this much of cooling effect by using vapor compression system with R134a refrigerant the system needs 321.3 kW of power considering a standard COP of 3.15. However, the vapor absorption system consumes only 26.2 kW, achieving net power savings of 295 kW. Therefore, if the produced cold duty is used within the plant to replace the cooling utilities produced by the vapor compression refrigeration system the overall thermal efficiency of the plant improves by 0.59% and finally reaches to about 58%.

At this point, further investigation could be carried out regarding other options of using the cold duty produced by the vapor absorption system. One possible way might be using the cold duty to cool down the inlet air temperature, which will increase the net power output of the plant as shown in Table 4.5.

In the absorption system, the cold stream temperature is about 3°C; therefore, we cannot cool down the air temperature below 8°C to maintain a minimum approach temperature of 5°C. The available cold duty from the vapor absorption system would be able to cool down the inlet air temperature from 25°C to 8°C and the excess cold duty, about 349.7 kW, could be used to provide support to the food storage or air conditioning system within the plant. The inlet cold air will decrease the gas turbine inlet temperature, thus the compressor pressure is increased to maintain our set temperature 1404°C at the gas turbine inlet to improve the system efficiency. This is due to the fact that at higher compression pressure the system becomes more economically and environmentally potential (Figure 4.8). Aspen HYSYS calculates the net power output of the system for this option as 29 MW and 58% system efficiency. The performance of this option is almost same as the other option. However, it will involve higher cost as it cannot utilize all the cooling utilities to cool down the inlet air temperature, therefore, the systems involved for the transportation of the excess cooling utility would add some extra cost. In this perspective, the first option would clearly produce more benefits. The designers may avoid the calculation of the IECP index as it is a simple study between two options and the cost benefit of the first option is obvious compared to the second option, while environmental performance for both options is almost same.

3.3.3.3 Application of Mass Integration

The main concern of the developed vapor absorption system is that it consumes a large amount of water which involves a significant amount of pumping power requirement. With mass integration, our target is to reduce the water usage in the system to reduce the power consumption. We investigated all the mass streams in the system and their operating conditions. The analysis indicates that the water used in the absorption system could be recycled via cooling down the temperature in the same column used for condenser water cooling system (Figure 4.15). In this case, the water temperature entering into the heat exchangers would be 23.9°C instead of 20°C because in the stripping column the water cannot be cooled down below the adiabatic temperature of the ambient air (23.9°C). The results of the mass integration are shown in the Table 4.11.

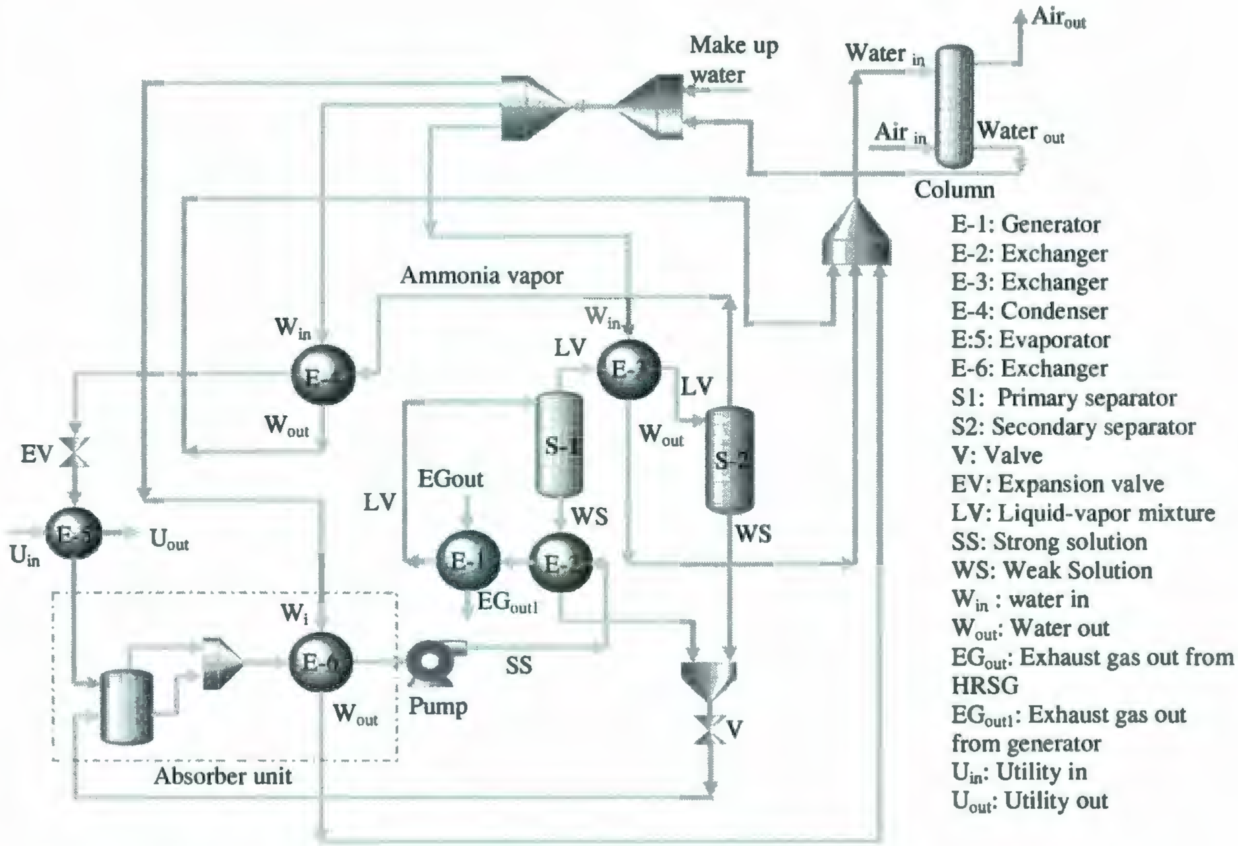


Figure 4.15: Vapor absorption refrigeration system with water recycling to column

Table 4.11: Characteristics of the Vapor Absorption Refrigeration System and the Whole Thermal System After Recycling the Cooling Water From Absorption Refrigeration System

Total make up water	26.5 ton/h
Utility in absorption system	207 ton/hour
Power input to pump	7.15 kW
Net power savings	23.2 kWh
Economic Benefits	$16,300
Overall efficiency	58 %

The table shows that due to the mass integration the amount of utility in the absorption refrigeration system increases from 125.9 to 207 ton/h which is due to the effect of cooling water temperature increase. Before the water recirculation from the absorption refrigeration system, the amount of total makeup water in the system was 23 ton/hour, which is increased by only 3.5 ton/h if utility water is recirculated. Due to this water recirculation, pumping power requirement in the absorption system is reduced to 7.1 kWh from 30.2 kWh (Table 4.10) giving a net savings of 23.2 kWh. The economic benefit from this power savings appearing in Table 4.11 is not very significant; however, if water treatment cost is included it will be considerably higher. Although CO_2 emissions/kWh will be almost unchanged, due to some economic benefits we choose this mass integration option in our flowsheet optimization activity.

3.3.3.4 Application of Heat Integration Tool

For applying heat integration the absorption refrigeration system is studied. The temperature and product of mass flow rate and heat capacity ($\dot{m}Cp$) of each stream is carefully analyzed to obtain possible matches between two process streams. The minimum approach temperature of 10°C is considered for this integration. Heat integration opportunity is identified between the stream (liquid vapor mixture) exiting the separator S1 and the stream leaving the heat exchanger E-2 before entering to the generator E-1 (Figure 4.15). The result of the heat integration is given in Table 4.12. The result shows that the COP of the absorption refrigeration system has been increased from 0.51 to 0.55. This is due to the effect of heat integration, which has reduced the use of external heat in the generator. Although in present case study we are using the waste heat, this heat integration has significance where external heat utility is used in the generator. In this case also, it may have meaningful role if the exhaust heat is decided to use further by employing the trigeneration.

Table 4.12: Characteristics of the Vapor Absorption Refrigeration System After Applying the Heat Integration

Total make up water	26.5 ton/h
Utility flow in absorption system	203 ton/hour
Power input to pump	7.5 kW
Waste heat used	1833 kW
Cooling effect produced	1004 kW
COP of the system	0.55

The result shows that the COP of the absorption refrigeration system has been increased from 0.51 to 0.55. This is due to the effect of heat integration, which has reduced the use of external heat in the generator. Although in present case study we are using the waste heat, this heat integration has significance where external heat utility is used in the generator. In this case also, it may have meaningful role if the exhaust heat is decided to use further by employing the trigeneration.

In Table 4.12, it is observed that the use of make up water in the plant remains almost unchanged; however, the amount of recycled water has been reduced by 4 ton/h. From this observation one can draw an important conclusion that due to heat integration the mass requirement in the system also might be changed. In case of heat integration, the only drawback is that it needs an additional heat exchanger E7 (Figure

4.16). In the next step with the help of the IECP index the impact of heat integration is studied.

For this, trigeneration is applied to use the exhaust heat leaving from the generator to produce some hot water utility for internal use within the power plant. In this case, the heat integration saves 80 kW of heat duty. The calculated IECP index for heat integration option compared to the base option is 0.027, which indicates that that heat integration option is slightly better.

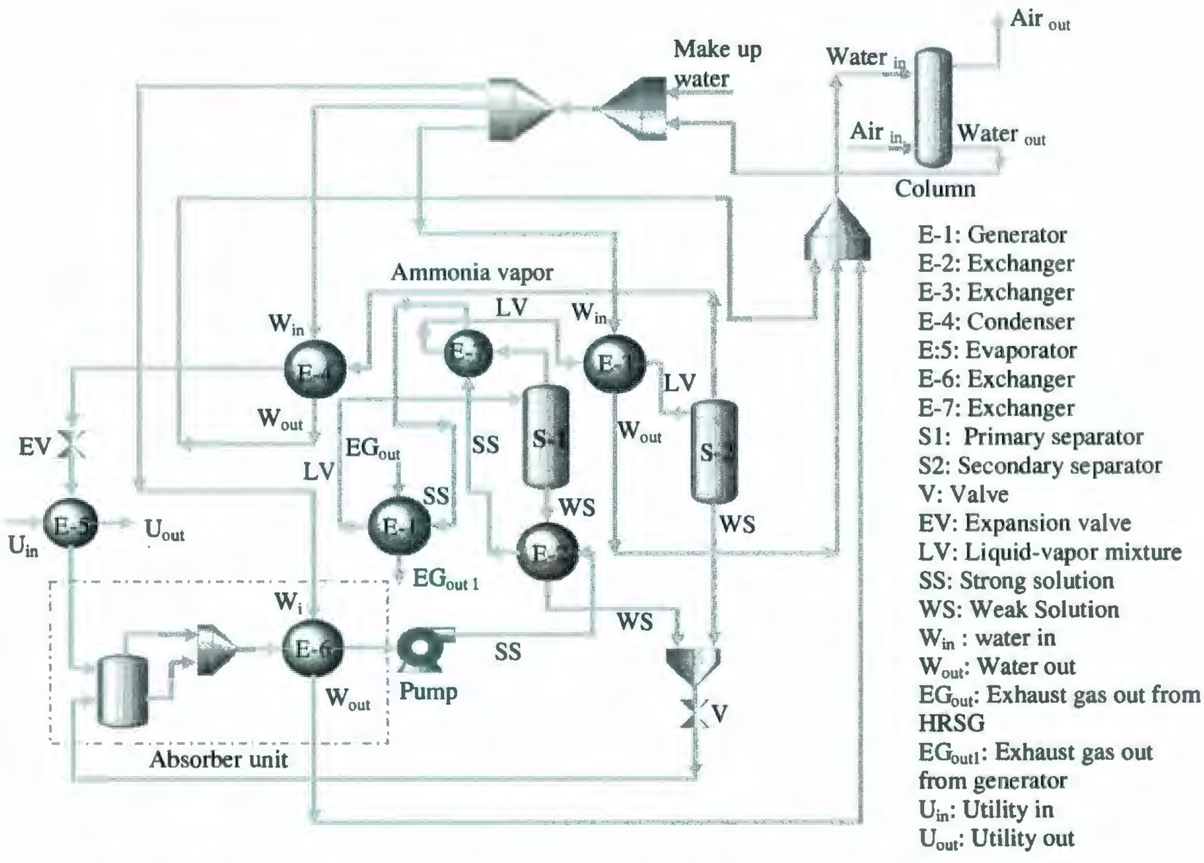


Figure 4.16: Vapor Absorption Refrigeration System after Heat Integration

3.3.3.5 Recalculation of Exergy and Energy

According to our proposed optimization approach, at this point, one needs to recalculate of the exergy and energy of the stream finally leaving the system boundary, i.e. from generator of the absorption system. The values of waste exergy and energy are 0.855 MW and 5.04 MW respectively.

3.3.3.6 Reapplication of Cogeneration/Trigeneration

The calculation shows that the energy value is still significant as compared to the exergy value. The calculated exergy is the aggregate of the thermo-physical and chemical exergy. The thermo physical part is about 266 kW and rest is the chemical exergy which cannot be easily converted to useful work. However, this stream could be still used due to having some exergy value to produce some hot utility at a minimum approach temperature of 10°C. We have decided to use this heat to heat up the water for process need in another small process industry installed in the same premises.

The simulator shows that an additional 4169 kW heat could be used to heat up 151 ton/hour water from a supply temperature of 20°C to 43°C, while the exhaust gas will cool down to 30°C. If this heat is produced via consuming electricity from the same power plant having 58% efficiency, the additional 7187 kW power would be required. Therefore, the efficiency of the whole system due to this trigeneration will be improved to 66.4% and the CO_2 emission would be reduced to 0.3 kg/kWh. Since this heat recovery does not involve much cost, the total annualized cost/kW-year would also be reduced significantly which would make this option very attractive.

3.3.3.7 Reapplication of Mass/ Heat Integration Tool

According to the our optimization approach for the developed flowsheet (Figure 4.17), mass integration and heat integration opportunity should be reviewed, however in this case they could not be applied.

3.3.3.8 Recalculation of Exergy/energy

The exergy and energy are again calculated for the stream leaving finally from the system. The exergy and energy values are calculated as 621 kW and 835 kW respectively. The thermo-physical part of the exergy is only 9.4 kW. This clearly indicates that energy could not be recovered from the stream practically due to its low exergy value, so structural optimization is not further possible and parametric optimization needs to proceed. The final structure of the flowsheet developed using SusDesign approach is shown in Figure 4.17.

3.3.4 Parametric Optimization of Each Unit

Table 4.9 shows that the highest exergy destruction occurs in the furnace and then in the HRSG. The exergy destruction in steam turbine, gas turbine and air compressor is

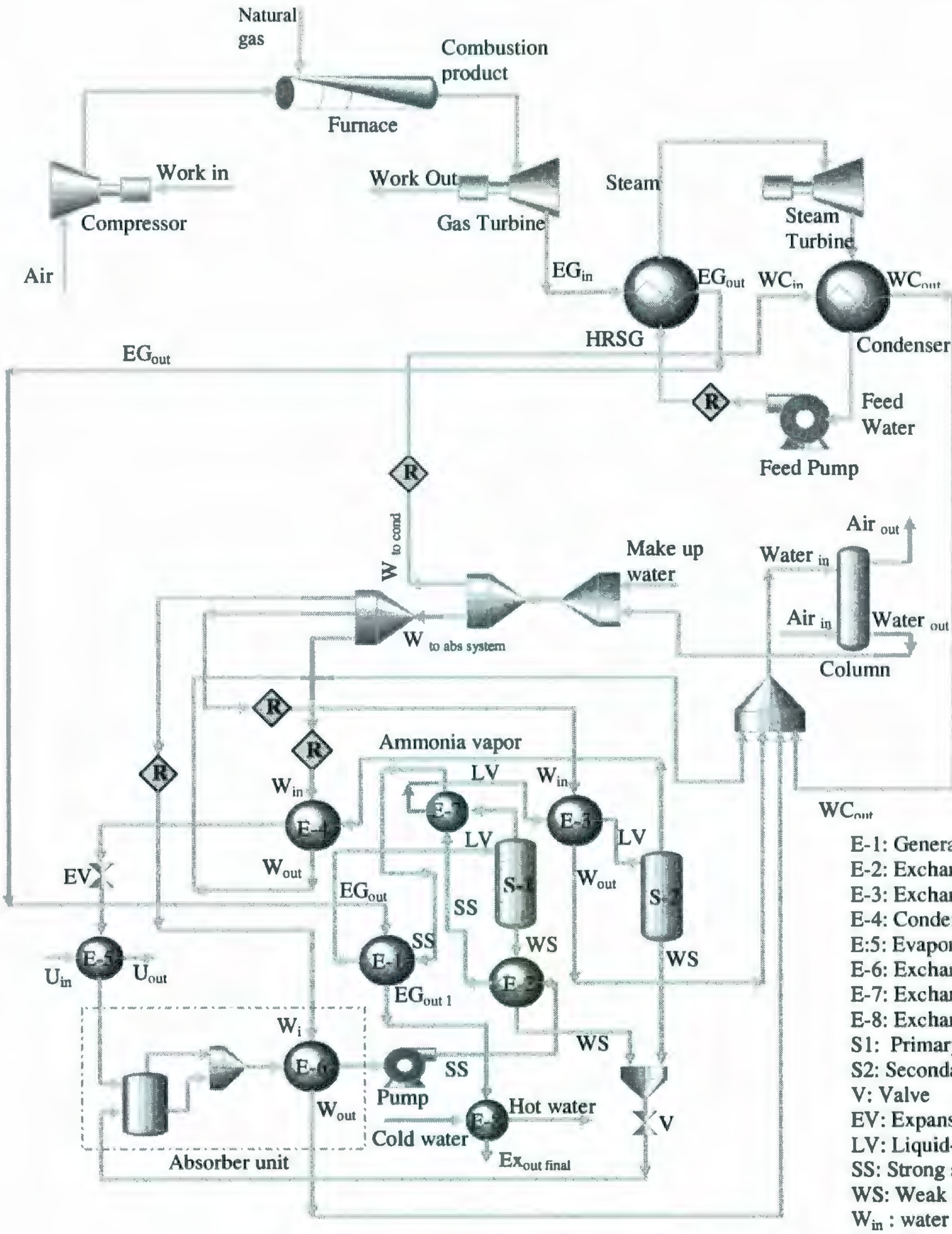


Figure 4.17: The Complete Design of Proposed Thermal System

E-1: Generator
E-2: Exchanger
E-3: Exchanger
E-4: Condenser
E:5: Evaporator
E-6: Exchanger
E-7: Exchanger
E-8: Exchanger
S1: Primary separator
S2: Secondary separator
V: Valve
EV: Expansion valve
LV: Liquid-vapor mixture
SS: Strong solution
WS: Weak Solution
W_{in} : water in
W_{out}: Water out
EG_{out}: Exhaust gas out from HRSG
EG_{out1}: Exhaust gas out from generator
U_{in}: Utility in
U_{out}: Utility out

also significant. Therefore, to reduce the exergy destruction from the system, these unit operations need to be investigated thoroughly. The parametric optimization is an effective way that allows minimization of the entropy generation within the processes by reducing the irreversibility and thereby reducing the exergy destruction. The parametric optimization of different significant units has been carried out sequentially according to Figure 4.18.

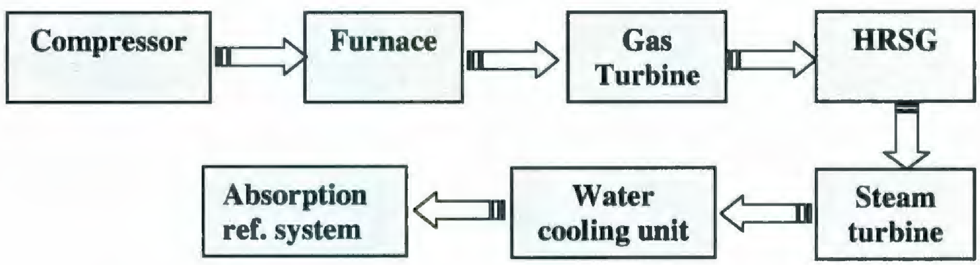


Figure 4.18: Sequence of Parametric Optimization of Different Units

To reduce the exergy destruction in the compressor, the sensitivity analysis is carried out by Aspen HYSYS to investigate the effect of isentropic efficiency on the exergy destruction. It is observed that exergy destruction reduces linearly with the increase of the isentropic efficiency, which consequently increases the net power output of the plant and reduces CO_2 emissions/kWh. The higher isentropic efficiency increases the fixed cost of a compressor for a given kW capacity, however decreases the operating cost due to the increased power output. For optimizing the compressor unit, IECP index for different isentropic efficiency options are calculated.

The IECP calculation method has been set up in the optimizer spreadsheet. When optimizer runs, with the change of isentropic efficiency the IECP value for the corresponding option is calculated. Due to the increase in isentropic efficiency the gas turbine inlet temperature is reduced for a particular pressure. Therefore, in order to optimize the performance of the thermal system the pressure of the compressor is varied to keep the gas turbine inlet temperature constant. The design of the optimization is shown in Table 4.13.

Table 4.13: Optimization Design for Air Compressor

Objective function:	IECP to maximize
Isentropic efficiency varied between:	80 – 90%
Compressor pressure:	1100 -1500 kPa
Constraint functions:	
Gas turbine inlet temperature	< 1402°C
Total operating cost	< 5 cents/kWh

It is important to note that in order for optimizer to converge quickly the range of the decision variables should be narrow. The previous study on the selection of the potential pressure options shown in Figure 4.8 provides the basis to narrow down the pressure range. Table 4.14 shows the optimization results, the optimum value of IECP index is obtained for 90% isentropic efficiency and 1307 kPa compressor exit pressure option. The base case for this optimization is considered as 85% isentropic efficiency and 1200 kPa compressor exit pressure. The optimum option improves the overall system efficiency from 66.4 to 66.8%.

The performance of the combustion greatly depends on the residence time in the furnace and the value of λ. The sensitivity analysis is carried out to study the effect of different values of λ on exergy destruction for the previously set residence time of 1.98 sec. The result is shown in Figure 4.19.

Table 4.14: Results of the Air Compressor Optimization.

Isentropic Efficiency	Pressure kPa	IECP
90	1307	1.429
90	1293	1.38
90	1293	1.34
90	1293	1.32
90	1292	1.31
90	1292	1.31
88	1251	1.00
87	1220	0.68
87	1220	0.68
86	1200	0.48
87	1160	0.39
86	1140	0.19

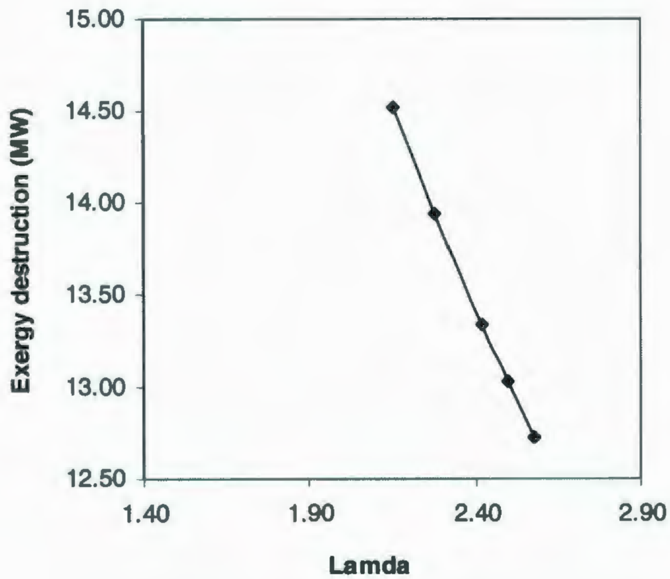


Figure 4.19: The Effect of λ on the Exergy Destruction in the Furnace.

The figure shows that exergy destruction strongly depends on the λ value, for higher λ values destruction becomes lower. Previously, in Figure 4.7 it was observed that λ of 2.15 was the optimal option, however, from exergy perspective, Figure 4.19 shows that the options with higher λ values have more potential. Since the furnace has serious interactions with other unit operations, the overall optimization would be the better option to take into account the effects of such interactions. The sensitivity analysis result in Figure 4.19 gives a basis to set up a narrow range for λ during the optimization.

For the optimization of the gas turbine, isentropic efficiency is varied from 85 to 90%, and the operating cost ≤ 5 cent/kWh is set up as a constraint. The result of the optimization is shown in Figure 4.20. From the figure it is obvious that 90% isentropic efficiency is the best option within the investigated options and for this option overall system efficiency improves to 68% from 66.8%.

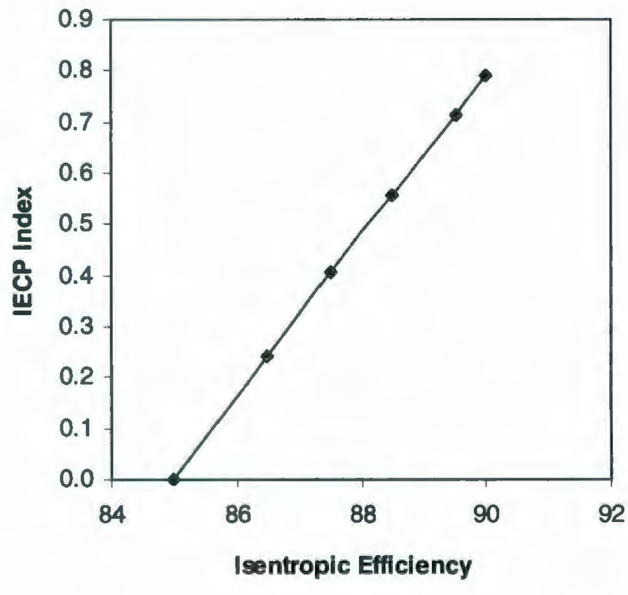


Figure 4.20: Results of the Optimization for Gas Turbine

The exergy destruction in any heat exchangers greatly depends on the minimum approach temperature. The sensitivity analysis is performed to investigate the effect of the minimum approach temperature on the exergy destruction in the HRSG unit. The result is shown in Figure 4.21. The figure shows that exergy destruction decreases with the decrease of minimum approach temperature. To reduce the minimum approach temperature, the difference between gas turbine outlet temperature and steam temperature should be low, which could be easily achieved by producing higher temperature steam.

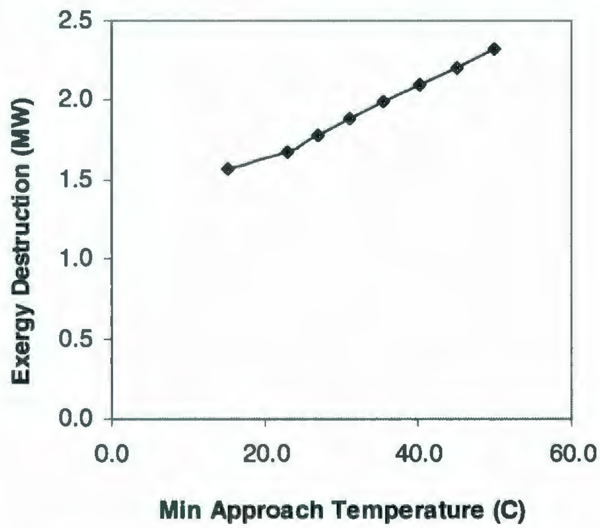


Figure 4.21: Effect of Minimum Approach Temperature on Exergy Destruction in the HRSG

For low minimum approach temperature, the cost of the HRSG increases due to the increase of the heat transfer area and the requirement of high temperature resistant material. On the other hand, lower minimum approach temperature increases the net power output of the plant due to the minimization of exergy destruction and thus reduces the emissions/kWh. In order to get the optimum option, the IECP index for different minimum approach temperature options is calculated and the option with the maximum index value is selected by the Aspen HYSYS optimizer. Figure 4.22 shows the optimization results for HRSG; the optimum option is selected for 10°C minimum approach temperature. Due to this optimization, the efficiency of the overall system improves from 68 to 68.9%.

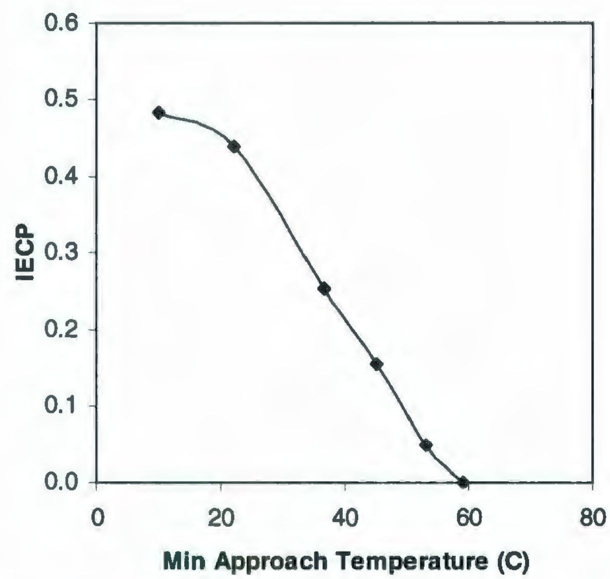


Figure 4.22: Results of the Optimization for HRSG

Similar to the gas turbine, the optimization of steam turbine is carried out by varying the isentropic efficiency and the option having the maximum IECP index is selected. Figure 4.23 shows the optimization results; it shows that that the option with 90% isentropic efficiency is the optimum in terms of the combined environmental and economic viewpoint. For the optimum option, the efficiency of the thermal system improves to 70%.

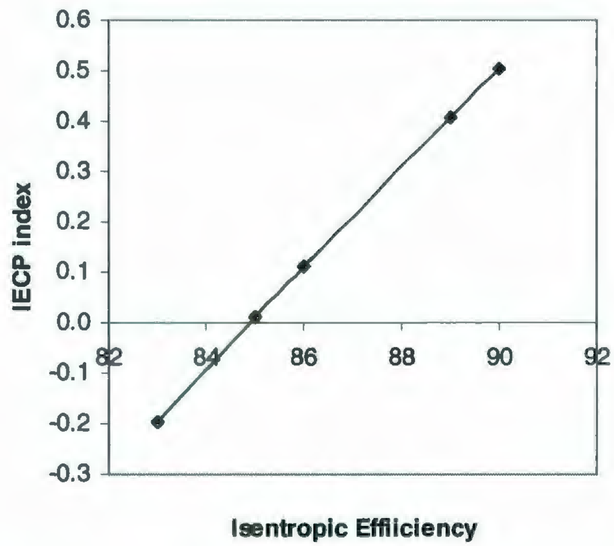


Figure 4.23: Results of Optimization for Steam Turbine

The main target of the optimization of water cooling unit is to reduce the make up water requirement. This optimization study is based on the parametric optimization of all important parameters. The optimization design is given in Table 4.15.

Table 4.15: Optimization Design for Recycled Water Cooling Unit

Objective Function:	Make up water to maximize
Air amount:	Vary between: 1500 to 3000 T/h
Column Ist stage pressure:	92 to 98 kPa

After the optimization is completed, the make up water is reduced from 26.5 ton/h to 26 ton/h and the optimum parameters are set as 1800 ton/h air flow and 98 kPa column (Ist stage) pressure. The optimization results in the reduced air flowrate which reduces the power input to the air blower.

The purpose of optimization of the absorption refrigeration unit is to improve the coefficient of performance of the system by selecting the optimum operating parameters. The design of the optimization is presented in Table 4.16.

Table 4.16: Optimization Design for Absorption Refrigeration System

Objective Function:	COP - maximize
Absorption pressure	Vary between: 460 - 490 kPa
Condensation pressure	Vary between 1200 - 1240 kPa
Molar flow of ammonia water solution	Vary between 700 - 820 kgmol/h
Molar flow of ammonia vapor	Vary between 460 - 490 kgmol/h

As a result of the optimization the COP improves from 0.55 to 0.56 and the defined operating parameters are shown in Table 4.17.

Table 4.17: Optimum Operating Parameters for Absorption Refrigeration System

Absorption Pressure:	478 kPa
Condensation Pressure:	remain unchanged
Molar flow of ammonia water solution:	818.8 kgmol/h
Molar flow of ammonia vapor:	193.7 kgmol/h

3.3.5 Overall Optimization of the Thermal System

This is the last step of a preliminary process design. At this stage, the whole thermal system is optimized in order to consider the interaction effects among different unit operations. The sensitivity analyses performed so far at different stages of the design help to identify the important operating parameters for different units and setting up a narrow range for each parameter to lay out the optimization design. The overall optimization design is given in Table 4.18.

Table 4.18: Design of Overall Optimization of the Proposed Thermal System

Objective function	**IECP** to maximize
Primary variables	**Range**
Adiabatic efficiency for compressor, gas turbine and steam turbine	88 – 90%
Compressor delivery pressure	1100-1800 kPa
Value of λ	1.95 – 2.34
Steam temperature	680 – 720°C
Steam pressure	180 – 210 bar
Constraint Functions:	
Turbine inlet temperature	< 1410°C
Cost/kWh	< 5 cent

The flow sheet developed so far is considered as the base case for this optimization. The optimization improves the environmental and economic performance very insignificantly by reducing only the value of λ to 2.13 keeping other operating parameters exactly same as the base option. The IECP value of the optimized flowsheet is obtained as 0.03, which indicates that the overall optimization improves the combined economic and environmental performance very insignificantly. This is due to the fact that because of the systematic use of SusDesign approach, the cost and environmental performance of the flowsheet has been optimized gradually and thus, further scope for optimization has been narrowed down.

4.0 Conclusions

The proposed SusDesign approach has been successfully applied in designing a thermal power plant. The application of this approach has finally developed an efficient, cost effective and environmentally friendly thermal system design. The developed design has achieved an overall thermal efficiency of 70%, CO_2 emissions about 0.28 kg/kWh and NO_x emissions about 0.2 g/kWh; while in a typical natural gas fired power plant the thermal efficiency varies in the range of 23-36%, emissions of CO_2 is about 0.54 kg/kWh, NO is about 1 g/kwh (Polyzakis et al., 2008; Miller and Atten, 2004). The cost of per kWh power generation is estimated as 4 cents, which is also reasonably low compared to other power plants.

Through this case study, it is experienced that the approach is easily applicable; especially the integration of IECP tool with Aspen HYSYS provides strong computational support to carry out the analysis, evaluation and screening of alternatives for selecting the optimal options at every level of process design.

The case study also shows that the application of SusDesign approach has improved the environmental and economic performance of the design gradually throughout different design stages and makes it nearly optimal. Therefore, during overall optimization very insignificant improvement has been noticed.

The SusDesign approach is applicable to design a wide variety of process systems. Although in present case study, it has been successfully applied to a thermal process system design, more case studies need to be carried out to examine its wider applicability.

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Chapter 5

IECP- An Approach for Integrated Environmental and Cost Evaluation of Process Design Alternatives

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Preface

This manuscript chapter provides a detailed description of an approach to quantitatively evaluate a process design option based on an integrated environment and cost index. A version of this manuscript is submitted to the journal of *Energy for Sustainable Development* for possible publication.

The work described in the manuscript is a joint effort of the authors. The first author (Khandoker Hossain) initially developed the framework which was revised based on the suggestions of the co-authors (Drs. Khan and Hawboldt).

The first author designed a case study to demonstrate the applicability of the developed approach. He did the details of the case study which involved the modeling of different design options in the Aspen HYSYS, implementation of the approach, analysis and interpretation of results. The co-authors monitored the progress, reviewed the results and provided suggestions. The first author prepared the first draft of the manuscript which was revised based on the comments and suggestions of the co-authors.

Abstract

This paper proposes a methodology (IECP) for the integrated environmental and cost evaluation of a process design option. It is designed for quick quantitative evaluation of a design option at different levels of process synthesis or retrofit applications. A hazard based approach, Pro-hazard, has been developed for the quantitative evaluation of environmental potential of design options by using a cradle-to-gate life cycle assessment. This assigns an environmental potential index, P2P, to a design option by comparing its environmental performance with respect to the base option. To quickly evaluate the cost of the resulting option a simple approach, Eco-index has been developed. It gives a cost potential index, CP, to a specific design option by comparing its unit operating and fixed cost with respect to that of the base option. In the IECP framework, both the P2P and CP indices for a design option are combined by assigning an appropriate weighting factor to each index, which gives an integrated environmental and cost potential index, IECP, for the design option.

In this paper, IECP methodology has been combined with a process simulator, Aspen HYSYS, to obtain the necessary data to quickly and accurately determine the IECP index. The applicability of the proposed IECP approach has been demonstrated through a case study for the selection of potential NOx prevention options in a 125 MW combined cycle power plant from a large number of options related to flue gas recirculation, steam and water injection to the furnace.

Keywords: Cost, Environment, Index, Process design, NOx.

1.0 Introduction

Process industries are the main concern for rapid degradation of environmental quality. In order to achieve sustainability, green as well economically viable process design is today's greatest challenge. In conventional process design and synthesis, environmental issues are addressed by adopting control technologies, which are not capable of achieving environmental as well as economic sustainability.

A significant amount of work has been dedicated to incorporate environmental issues during the early stages of the process design (Azapagic et al., 2006, Dantus and High, 1996; Ciric and Jia, 1994; Crabtree and Elhalwagi, 1995; Gupta, and Manousiouthakis, 1994; Dunn et al., 1993; Richburg and Elhalwagi, 1995; Douglas, 1992). As a design objective most identify cost, and consider environment as a design constraint (Cano-Ruiz and McRae, 1998). Even in the recent process design books there are no clear guidelines as to how to incorporate environmental issues as design objective (Cano-Ruiz and McRae, 1998).

In a few cases, the environmental performance is only evaluated when a complete flow sheet is developed (Azapagic et al., 2006; Young and Cabezas, 1999; Cabezas et al., 1999, Stefanis et al., 1995; Pistikopoulos et al., 1995). This cannot insure the design is optimum from an environmental viewpoint.

Some studies have used a more robust approach to incorporating environmental issues during the preliminary stage of process design. The environment is identified as one of the design objective functions at each and every level of a process flow sheet synthesis (Douglas, 1992; Lewin, 2000; Alexander et al., 2000). The cost is evaluated quantitatively at each level of synthesis, while the environment is evaluated qualitatively. As a result, the selection of the most environmentally benign options cannot be guaranteed. Quantitative evaluation of economics has been well studied and methodologies are present in the literature, However, a simple approach for quantitative environmental evaluation of design options at different stages of process synthesis is not available in the literature.

For multi-objective environmental impact evaluation, use of an overall single indicator is a popular method (Hossain et. al., 2007; Goedkoop, 1995; Goedkoop and Spriensma, 1999; Young et al., 1999). Khan et al., (2004) developed an integrated single index by considering three process design objectives, i.e., environment, safety and cost, and applied to a case study for selecting the best fuel option in a power generation system. The method is qualitative and designed for the detailed analysis of a developed flowsheet.

There is a lack of adequate approach to determine an integrated index considering cost and environment for the quick evaluation of process alternatives generated at different steps of process synthesis.

In this context, the present paper has proposed a quantitative tool, IECP, for developing an integrated environmental and cost index. It has the following attributes:

i) It could be set up in a process simulator for performing quick screening, evaluation, and optimization of design alternatives at every level of process synthesis.

ii) Through a two step screening process it insures the selection of the potential design options for further design considerations.

iii) For environmental impact evaluation of design alternatives, it splits the cradle-to-gate life cycle system boundary into two domains, cradle-to-gate and gate-to-gate domain, which would help with assessing the impacts of each domain separately.

iv) For developing both the cost and environmental indices, normalization is done by adopting a simple ranking method, which provides a strong basis to integrate both indices to get an integrated overall index.

In the present paper, the applicability of the proposed IECP approach has been demonstrated through a case study for selecting the NOx prevention alternatives with most potential in a 125 MW combined cycle power plant.

2.0 Description of IECP Approach

The architecture of the IECP approach is shown in Figure 5.1. The application of the IECP approach generates only the potential options for design consideration. The description of different major steps of the IECP approach is given below.

2.1 Select a P2/design option

Prior to the application of IECP approach, the designers must first generate design options at a particular stage of process synthesis. This is typically done through "experience" or a process design methodology such as our proposed SusDesign, Douglas hierarchy, etc. (Hossain et. al., 2009; Douglas, 1992).

2.2 Collect/Predict the Emission data

At this step, designers need to collect data on different emissions associated with the options. Data could be collected through literature search, pilot scale experiments or from existing plants. In case of lack of raw data, the designers may model the process using a process simulator and predict the emissions.

2.3 Screening the Options

In this step, the emission data on each component for a design option is compared with the corresponding regulatory limit. In case of the lack of regulatory data, the designer may set a limit based on experience or specific situation. The options that fail to comply the regulatory limit will be screened out and those that do comply will proceed further for environmental and cost potential evaluation. This initial screening insures that the selected options are environmentally sound and saves a significant amount of design time.

2.4 Estimation of P2 Potential Index

This step is concerned with the evaluation of environmental performance of design options by using the developed hazard based approach, Pro-hazard. It can quickly evaluate the environmental performance of different design options by determining a numerical index (P2P) for each option which will be discussed later in this paper.

2.5 Estimation of the Cost Index

In this step, the economic performance of the potential design options is determined by assigning a numerical index, CP, to each option. For determining the CP, the developed Eco-index method has been used, which will be discussed later.

2.6 Determination of the IECP Index

The purpose of this step is to determine an integrated index by combining the cost and environmental potential indices of any design option. It would provide a basis to compare different design alternatives based on a single overall index, IECP. The value of IECP index depends on the weighting factors, w_1 and w_2. The weighting factors indicate that how much importance will be given to a particular objective. Assigning of the weighting factors is the most controversial part; so far there is no accepted approach for this (Goedkoop and Spriensma, 1999). The value of the environmental weighting factor, w_1, depends on the plant specific scenario, like distance of the nearest population, background risk in the vicinity, the common emissions from the plants, present environmental regulations and future trend associated with the emissions from the plant. Furthermore, the predicted risk to the workers' health and the associated health cost are also important to consider determining the weighting factors for the environment. For assigning the weighting factor w_2, for CP, one needs to consider the predicted profitability criteria over the service life of the plant, such as net annual income return on investment, payback period and so on.

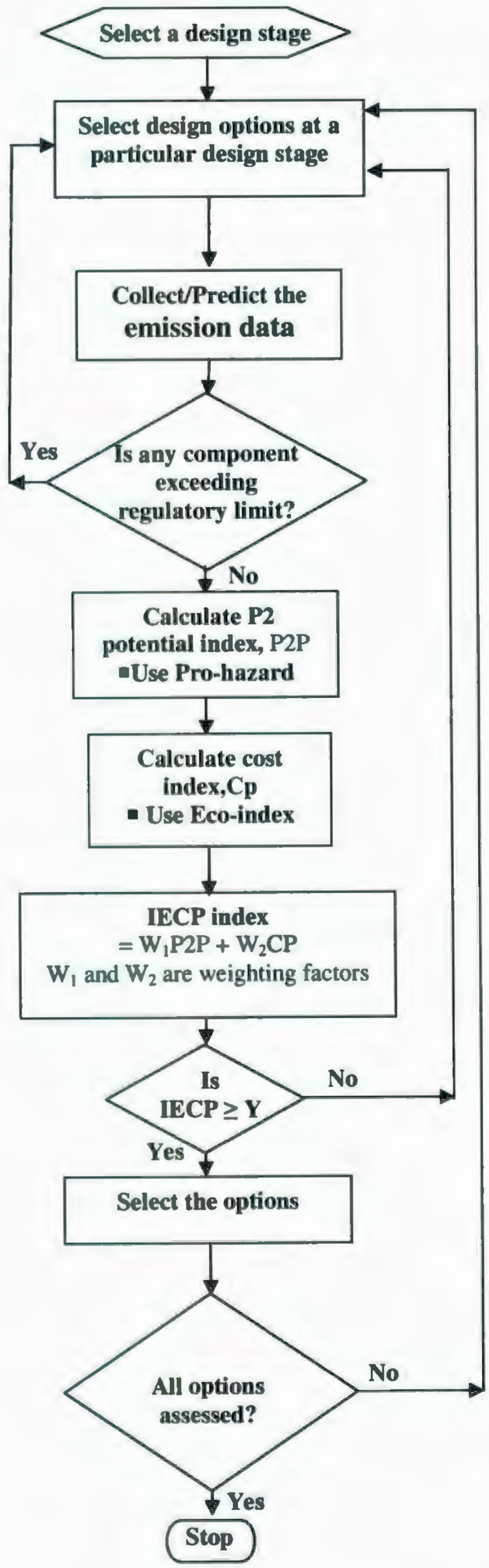

Figure 5.1: Architecture of the Integrated Environmental and Cost Potential Index Quantification Approach

In the next step, the IECP index for each design alternative is compared with the predefined value Y. This will screen out inefficient options and identify options with higher potential for further design considerations. Since in the preceding step, all the design alternatives have been passed through an environmental screening process, the options screened out at this step are the ones which do not have the cost potential. This understanding would provide a direction of improvement for the screened options. In this way, it does not only identify the potential design alternatives, but also assists the designer to improve a specific option.

The value of Y should be assigned by the designer by considering the value of w_1 and w_2 and the design target. The number of the alternative options to be selected at each level of process synthesis depends on the assigned value of Y; the higher the value of Y, the lesser the short listed options. The higher value of Y insures that the design is more robust on environmental and cost considerations.

3.0 Pro-hazard Approach

As mentioned in the previous section, Pro-hazard is a tool that determines the environmental performance of any design alternative by assigning a numerical indicator. The purpose of this tool is to provide a quick quantitative environmental evaluation, which is crucial for the decision support during preliminary process design, where only few potential options are selected from a large number of options at each step of design.

Pro-hazard evaluates environmental impact based on a hazard based approach, which is relatively quick and simple. Furthermore, hazard index database for a wide range of chemicals are available (Cabez et al., 1999, EPI, 2001; IRCH, 2004; Davis et al., 1994). The framework of the Pro-hazard approach is shown in Figure 5.2.

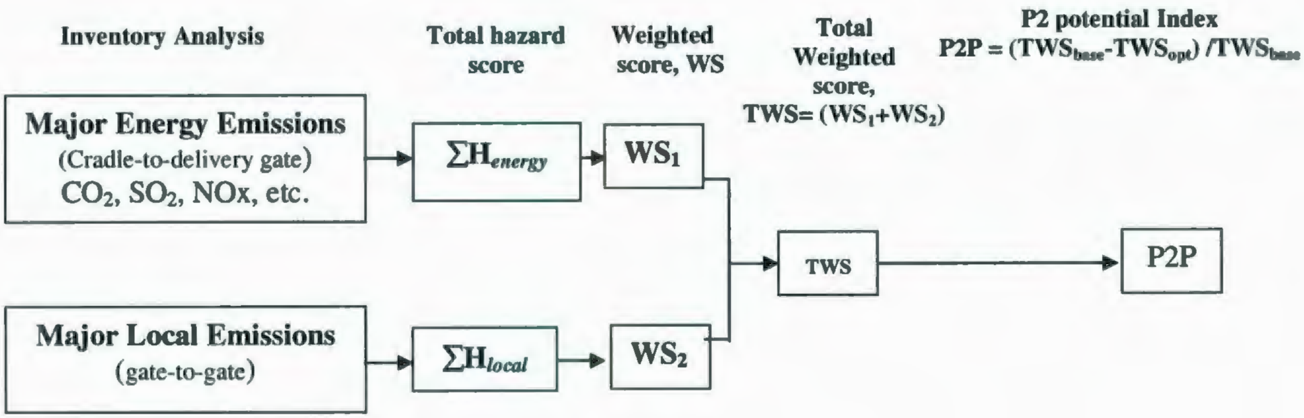

Figure 5.2: Framework of Pro-hazard Approach

The important aspect of this method is that it considers the cradle-to-gate system boundary which is split into two domains: cradle-to-gate domain and gate-to-gate domain. This allows one to consider different emissions and assign different degree of emphasis to the impacts across the domains, which gives the flexibility to weigh local and global impacts of any options separately. Thus, the selected option based on Pro-hazard approach would be environmentally benign from both global and local environmental viewpoints (Hossain et al., 2007). The description of different steps of the Pro-hazard approach is given in following sections.

3.1 Inventory Analysis

In this step, the detailed inventory analysis is performed for each domain. Cradle-to-gate domain encompasses all the processes starting from minerals extraction, processing, raw materials production and transportation up to the plant receiving gate. In contrast, the gate-to-gate domain considers all the processes related to the material handling, processing, manufacturing of the product, packaging and transportation to the warehouse for final delivery. Therefore, the emissions in the gate-to-gate domain are very important from the viewpoints of workers' and local population health. On the other hand, emissions outside of the plant boundary are mainly responsible for damaging environmental air quality, such as global warming, acid rain, photochemical smog, ozone layer depletion, etc. These are called global effects of the emissions. The global effects are mainly due to the energy related emissions, such as emissions of CO_2, SO_2, CO, NO_x, etc. Therefore, for quick evaluation, the inventory analysis in this domain will consider only energy related emissions and the emissions of any other toxic chemicals that cause a serious environmental concern. The energy consumption data for different processes and related emissions are available in different life cycle inventory databases.

The inventory analysis in the gate-to-gate domain considers the significant emissions that the workers are exposed to due to the materials handling, leakage of pipe line, valve, seal, etc., and chemical spill. Furthermore, it also includes any significant emissions through the stack. For the purpose of quick evaluation, only the emissions which have significant environmental impact need to be considered.

3.2 Estimation of the Hazard Score

The hazard index of a chemical is estimated based on its toxicity and some physical and chemical properties, such as biodegradability, atmospheric half life, dispersion coefficients, etc.

Typically the environmental impact evaluation using hazard based approach requires collecting the hazard score of a chemical for different impact categories and aggregating these scores for all the chemicals for a specific impact category over a particular domain (Hossain et al., 2008). The next task is to get the total hazard index for a domain by combining the aggregated hazard score of different impact categories by assigning an appropriate weighting factor to each impact category (ref: E-impact). The advantage of this approach is that one can put the appropriate weighting factors to different impact categories considering the specific scenario; however, it consumes a huge amount of time. Therefore, for a quick evaluation, in the present paper IRCH total hazard score is used; it is developed by Indiana Clean Manufacturing Technology and Safe Materials Institute at Purdue University (IRCH, 2004). The IRCH total hazard score is developed by integrating both human health hazard score and environmental hazard score of a chemical giving a separate weighting factor for each impact category. Therefore, through the use of IRCH total hazard score, one does not need to gather hazard score of different impact categories for a specific chemical, which leads to the simple and quick calculation of total hazard index over a particular domain.

3.3 Calculated Domain Specific Weighted Score

In this step, the total hazard score for each domain calculated in the preceding step is multiplied by a weighting factor. This gives the total weighted score for that domain. The weighting factor indicates the different degree of emphasis given to the impacts of a specific domain. As local emissions usually have higher impacts on human and ecological health, it should have more importance over the global emissions, i.e. emissions occurred in the cradle-to-gate domain. The value of the weighting factor for the impacts in this domain is fixed and not scenario specific. Whereas the value of the weighting factor for gate-to-gate domain is scenario specific, and is assigned depending on the distance of the nearest locality from the process industry, background risk, size of the sensitive population, presence of any endangered species, etc. For instance, if the location of a plant is far away from the population centre and it does not have any harmful effects on the terrestrial and aquatic ecosystem, then the values of the weighting factors for the both domains may be same (Hossain et al., 2007).

The weighting factors are usually assigned considering any of the following principles: gap between the current impact level and the target impact level, cost of the health care and evaluation of the expert. In Pro-hazard, the latter approach is used. Once the values of weighting factors are decided, they would remain unchanged and could be used for further environmental evaluation of design alternatives. In the next step, weighted indices from both domains are added together to obtain the total weighted index for a specific design option over the cradle-to-gate life cycle domain.

3.4 Pollution Prevention Potential Determination

Pollution prevention potential of an alternative design option is defined as the difference between the total weighted score (TWS) of the base option and the alternative option. When the difference is positive, the environmental impact of the base option is higher than the alternative design option. It indicates that the design alternative has some P2 potential compared to the base option; similarly, a negative value indicates that the base case is better than the design alternative. Since, the difference of TWS for two options will have a unit, in order to make it normalized the difference of TWS for both options is divided by the TWS of the base option, which gives the P2P index. The P2P index indicates how much a design option is environmentally better or worse with respect to the base option. It is worth mentioning that Pro-hazard uses a simple ranking method for normalization which is consistent and free from any biasing effect. This P2P index will be used for the IECP index calculation.

4.0 Eco-index Approach

The architecture of the Eco-index approach is shown in Figure 5.3. This approach is very simple and capable of giving quick cost estimation of a design alternative. This feature is particularly important for preliminary process design, when a number of design alternatives are usually required to be evaluated quickly at each level of process synthesis. The following sections describe different steps of the Eco-index approach.

4.1 Cost Considerations

In this step, different categories of costs are considered for the economic evaluation of a design alternative. For the proposed approach, the unit operating and fixed cost (UOFC) is considered as the basis for cost indexing. This is the simplest way to compare two design alternatives from economic viewpoint, especially when in both cases the amount of product is not same. UOFC is defined as the combination of fixed cost and the operating cost for a unit amount of product based on the present value of money.

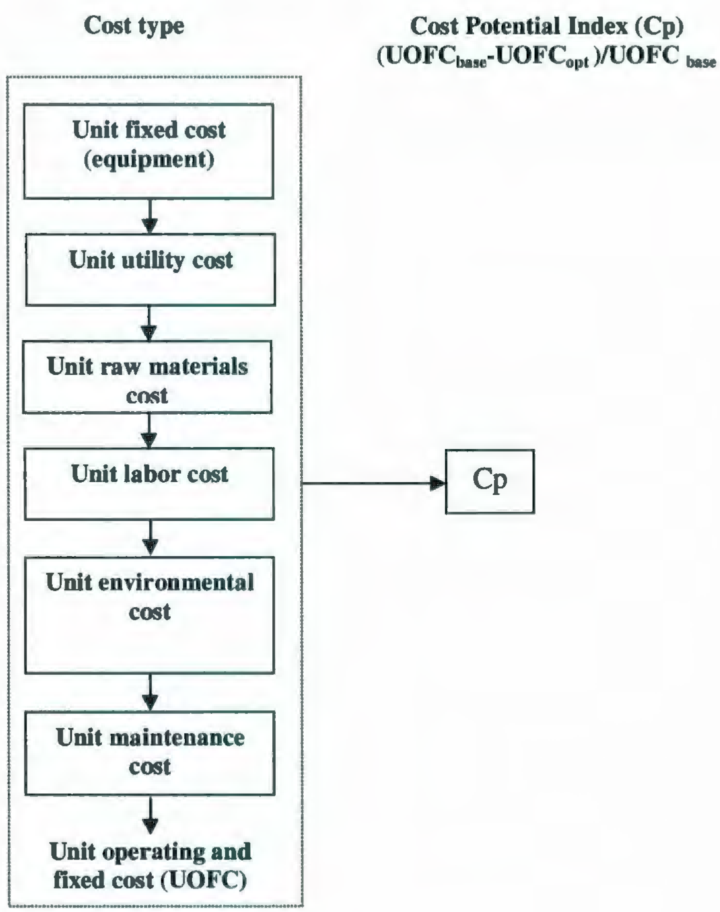

Figure 5. 3: Architecture of Eco-index Approach

Unit fixed cost is defined as the distributed cost over the service life of the project for a unit amount of the product. It can be expressed as follows:

$$\text{Unit Fixed Cost} = \frac{\text{Total Fixed Cost - Salvage Value}}{\text{Total amount of product produced over the service life}} \tag{5.1}$$

Salvage value is the estimated value of the project that will be realized at the end of its service life. The operating cost usually includes raw materials, utility, labor, maintenance and environmental costs. Sometimes the operating cost may include other costs as well, such as local taxes, insurance, administration costs, distribution and selling costs. However, in order to make the evaluation simple they were not considered for this method. Environmental costs include the costs related to the treatment of the waste, temporary storage of the waste, transportation, land filling, and deep well injection cost (Allen and Shonnard, 2002).

The breakdown of the operating cost in the Eco-index will help the designers to improve the economic performance of an option. This is especially important when designers want to improve an option that has good environmental potential but has been rejected only due to the poor economic potential.

4.2 Cost Potential Determination

Like P2 potential, cost potential of an option is defined as the difference of UOFC between the base option and the concerned option. A positive difference indicates the option has some economic potential with respect to the base option and a negative difference indicates the opposite. The cost potential of an option is normalized by dividing the UOFC of the base option, which gives the final cost potential index, CP. This indicates how much one option is better or worse with respect to the base option.

Since the value of CP for an option is mainly subject to the difference of UOFC of that option and the base option, if the cost of a particular category among the investigated options does not change significantly then the cost calculation for that category could be avoided.

As both the CP and P2P indices are calculated in the same manner, they could be used for calculating the integrated environmental and cost potential index (IECP). In both Pro-hazard and Eco-index approaches, a base case is considered for calculating the corresponding potentials. The base case could be the conventional design option or in the absence of a conventional option, the designers may declare any of the investigated design options as the base case.

5.0 Integration of IECP with Process Simulator

Quantitative evaluation of any process option is not straightforward, since it requires precise data and the obtaining of the data is not an easy task. Furthermore, the manual calculation of P2P and CP indices for each option involves a significant amount of time and effort. This could be easily overcome by integrating the IECP tool with a process simulator.

By modeling the process to be investigated, a simulator helps to carry out the economic and environmental analysis of each alternative option by examining the readily available data on equipment sizing, heat and power requirement, mass flow of raw materials and ancillary materials, consumption of utilities and mass separating agents, amount of product and waste, and the emissions of toxic chemicals.

As simulation runs the P2P and CP indices for different options are calculated with the aid of cost and environmental analysis data together with a set of cost and environmental functions. The values of P2P and CP indices are subsequently used for the calculation of IECP index for each option. The simulator compares the IECP index for different options with the set value of Y; this readily screens out the inefficient options and finally shortlists the options with higher potential. The choice of a simulator depends on the designers. In the present paper, the Aspen HYSYS process simulator is used.

6.0 Application of IECP tool

The IECP tool has been designed for a wide variety of processes; however, to demonstrate its use it has been applied to evaluate few NOx prevention alternatives during a thermal power plant design. The emission of nitrogen oxides (NOx) is a growing concern due to its detrimental effect on air quality. One of the major sources of NOx emission is thermal power systems (US EPA, 1999). In order to reduce its emission some preventive measures are considered at the design level by applying process modification strategies, which usually includes low NO_x burners, staged combustion, flue gas recirculation (FGR), reburning, water or steam injection, and low excess air firing.

In the present paper, different options of FGR, steam, and water injection were studied. FGR involves the recirculation of part of the flue gas into the air/fuel or combustion chamber prior to combustion. Usually the flue gas from the economizer outlet is recirculated either using exhaust fan/compressor and ductwork or induced directly using flow momentum of the flue gases. FGR reduces both the oxygen concentration in flame and peak flame temperature and thereby decreases the NO_x emissions.

Water injection (WI) is a widely applied technology for NO_x reduction in combustion devices. In principle, it is similar to flue gas recirculation. Water injection is especially effective for gas turbines; injection of water reduces the flame temperature since water becomes vaporized and eventually superheated taking heat from the combustion process. The steam injection (SI) is identical to water injection, where steam is injected instead.

In the present case study, a 125 MW combined cycle power plant was considered. The NOx emission was aimed to be reduced below 0.3 kg/MWh. The proposed IECP tool was set up in the Aspen HYSYS simulation environment and was used to evaluate different options of flue gas recirculation and water/steam injection and selecting the optimal options. For generating different NOx prevention alternatives a process simulator, Aspen HYSYS was employed.

6.1 Generation and Screening of Design Options

At this phase, different design options are generated which is followed by a screening process; both the generation and screening processes are carried out using Aspen-

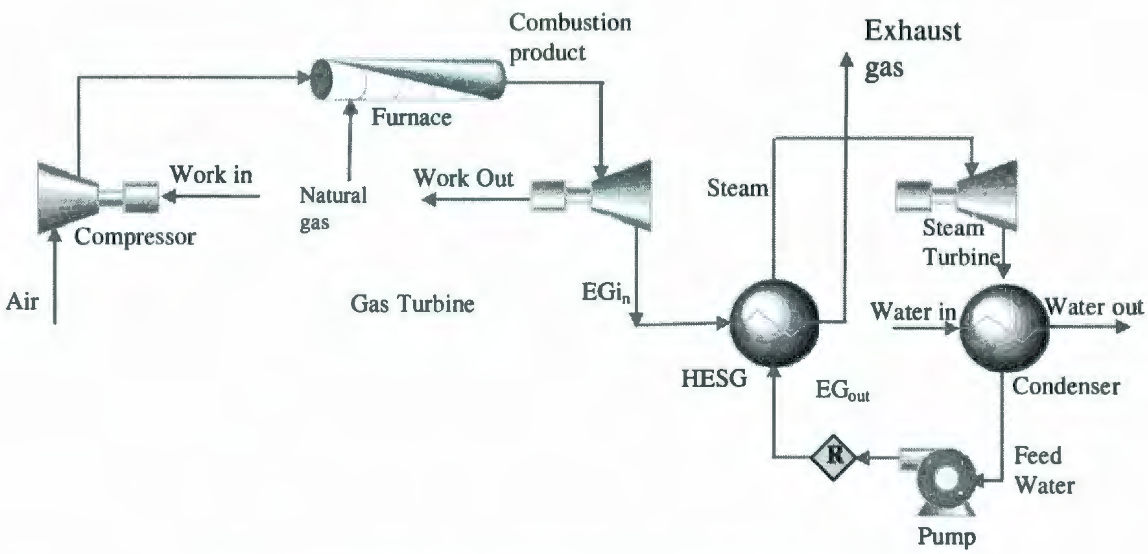

Figure 5.4: Schematic Diagram of the Thermal Power Plant

HYSYS. The behavior of NOx formation related to the power plant is important to be investigated to facilitate the generation of different options. In this study only thermal NOx has been considered and modeled using two steps kinetic reactions (Nicol et. al., 1999). The schematic diagram of the power plant considered is shown in Figure 5.4. The study was carried out for a range of combustion temperatures at (λ) of 2 and a combustion pressure of 1200 kPa. λ, is the ratio of actual air fuel ratio to the stoichiometric air fuel ratio. The results are presented in Figure 5.5, which show that as combustion temperature increases NOx formation also increases and the rate of formation is higher at higher temperatures. A portion of flue gas was recirculated from the exit of the heat recovery steam generator (HRSG) to the furnace, while keeping other operating parameters unchanged.

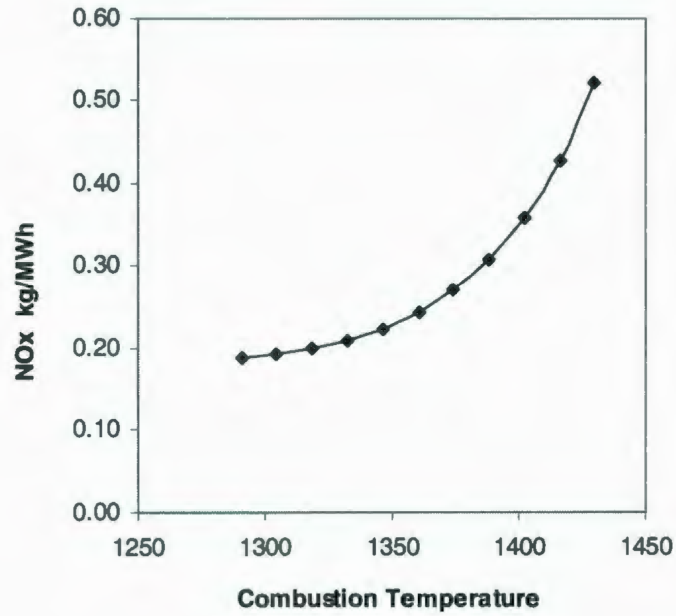

Figure 5.5: Effect of Combustion Temperatures on NOx Emission

For steam injection, some high pressure steam at 20 bar pressure was taken out from the steam turbine and injected to the furnace and for water injection, water at 25 °C was pressurized and injected through a nozzle. By using the process simulator, different options of flue gas recirculation and water/steam injection were generated and passed through a screening process to select the options that comply the set NOx emission limit of 0.3 kg/MWh. Table 5.1 shows different selected options of flue gas recirculation, water and steam injection respectively. The table also shows that below 10% flue gas recirculation and steam injection, the options were screened out, while in case of water injection, the invalid options were observed below 7200 kg/h of water injection.

Table 5.1: Different Options of Flue Gas Recirculation, Water injection and Steam Injection

Options	FGR (%)	WI kg/h	SI (%)
0	< 10 - screened out	< 7200 - screened out	< 10-screened out
1	10	7200	10
2	15	7500	15
3	20	7800	20
4	25	8100	25
5	30	8400	30

6.2 Estimation of P2P Index

In the next step, the P2P index for each alternative option was calculated from the emission data. As a base case, 15% flue gas recirculation option was considerd. The Pro-hazard was setup in the Aspen HYSYS spreadsheet to calculate the P2P index. The hazard index of different major components of the flue gas was collected from the IRCH data base and given as input in the spreadsheet. The values of IRCH index for CO_2 and NOx are 4 and 26 respectively.

According to the Pro-hazard approach, the total hazard index for different major flue gas components were calculated in both life cycle domains. In cradle-to-gate domain, the major emissions for the production and transportation of the required amount of natural gas to produce 1 MWh electric power was considered and for inventory analysis, Ecoinvent life cycle database was used (Ecoinvent, 2007). Only CO_2 emission was observed to be significant in this domain at 0.576 kg/MWh for 56% thermal efficiency of the plant. This value was multiplied by an efficiency correction factor and was considered as an input in the spreadsheet. This will facilitate the quantification of corresponding CO_2 emissions data while the efficiency of the plant changes with the change of design option.

For inventory analysis in the gate-to-gate domain, the emissions of different components for a specific design option were obtained by the simulator. The emission data of each component per MWh were multiplied by the corresponding IRCH total hazard index to obtain the total hazard index. For the present study, the weighting factor for the hazard in the cradle-to-gate domain was considered as 1, while double weight was applied to the hazard for the gate-gate domain. At first, the total weighted index (TWS) for the base option, i.e. 15% FGR option was estimated, which served as the reference value for estimating the P2P index for other options.

As an illustration, the TWS for 15% FGR option estimated by using Aspen HYSYS and Pro-hazard tool is presented in Table 5.2.

Table 5.2: The Calculation of TWS for 15% Flue Gas Recirculation Option

Major Emissions kg/MWh	**Total Hazard,** Index $\sum$Hi, i = 1 to n **kg/MWh**	**Weighted Score WS**	**Total weighted Score (TWS) kg/MWh**
Cradle-to-gate Domain	Cradle to gate domain		
CO_2 : 0.576	2.304	2.304	
Gate-to-gate domain	Gate-to-gate domain		2996.87
CO_2: 373	1497.28	2994.56	
NO_x: 0.2034			

Using the similar procedure, the TWS for 25% FGR option was calculated as 3052 kg/MWh and finally the P2P index for 25% FGR calculated with respect to the TWS of 15% FGR was -1.83. The negative index value signifies that the base case has better environmental potential than 25% FGR case.

6.3 Estimation of Cost Index

Once the P2P index for any option is calculated, the option will be further evaluated for CP index determination by employing the Eco-index approach. The cost functions of different equipment were developed from the available data using equation fitting technique, which was set up in the spreadsheet of the Aspen HYSYS. The cost functions include the variables that influence the cost of equipment such as pressure, temperature, equipment size, etc. For a particular option, the simulator provides the data of the variables required for cost calculation of different equipment. Similarly other costs such as environmental cost, maintenance cost and so on shown in the Eco-index framework are also calculated by the simulator with the aid of mass and energy balance data and a set of cost functions. According to the Eco-index approach, different costs have been calculated for a unit amount of product i.e. cost/MWh, which are subsequently added to obtain the total cost/MWh. In case of CP index estimation, the same option, i.e. 15% FGR, was considered as a base option for maintaining the consistency.

6.4 Estimation of IECP index

To estimate the IECP index both the CP and P2P indices were combined in the Aspen HYSYS spreadsheet with the appropriate weighting factors. In the present case study, equal weight was considered for both indices. Once all the functions and constants were properly defined in the Aspen HYSYS simulation environment, the IECP index for different options were readily calculated by the simulator as simulation ran. The IECP index values for different FGR, water/steam injection options are shown in Figures 5.6-5.8. Figure 5.6 shows the IECP index for different flue gas recirculation options.

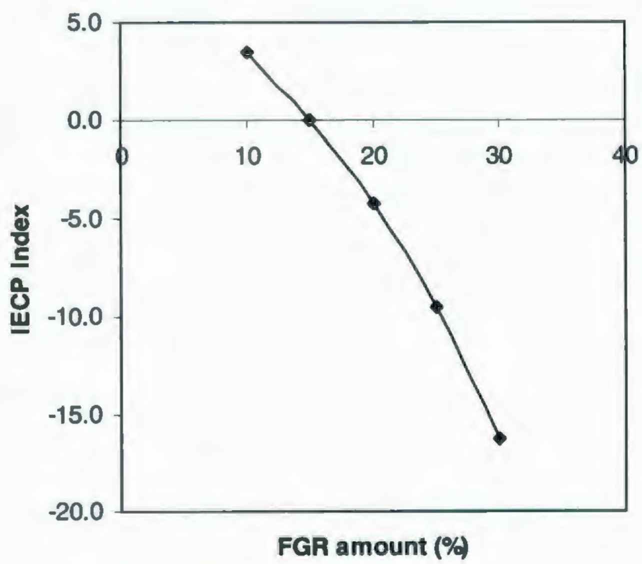

Figure 5.6: IECP Index for Different Flue Gas Recirculation Options

The figure also shows that only one FGR option is better compared to the base case, i.e. 15% FGR option. The increased amount of recirculation from the base case results in lower IECP index. Table 5.3 shows that as the amount of FGR increases, the NOx emission decreases, thus one may think that for increased amount of recirculation the P2P index may increase and that may improve the IECP index. However, because of the increased amount of recirculation the plant net power output decreases due to the more power consumption in the flue gas delivery compressor that increases the UOFC and the CO_2 emission for unit power output (Table 5.3). Therefore, for higher FGR options, despite of having some benefits due to less NOx emissions, the cumulative effect of cost and CO_2 increase ultimately results in the lower IECP index.

Table 5.3: Emissions of CO_2 and NOx for different FGR options

FGR amount (%)	CO_2 emission kg/MWh	NOx emission kg/MWh
10	359	0.220
15	363	0.191
20	368	0.182
25	373	0.180
30	381	0.183

Figure 5.7 shows that the IECP index for all the investigated water injection options are negative, which indicates that they are worse than the base case from the combined environmental and cost aspects. The IECP index for different investigated steam injection options are shown in Figure 5.8. It is observed that only two options,

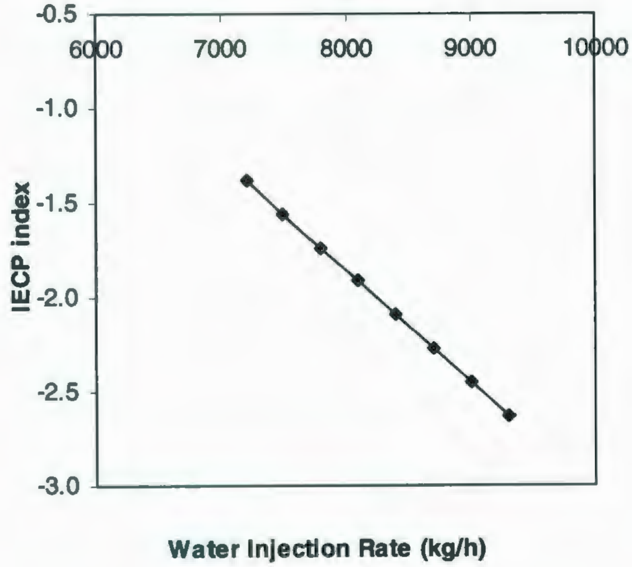

Figure 5.7: IECP Index for Different Water Injection Options

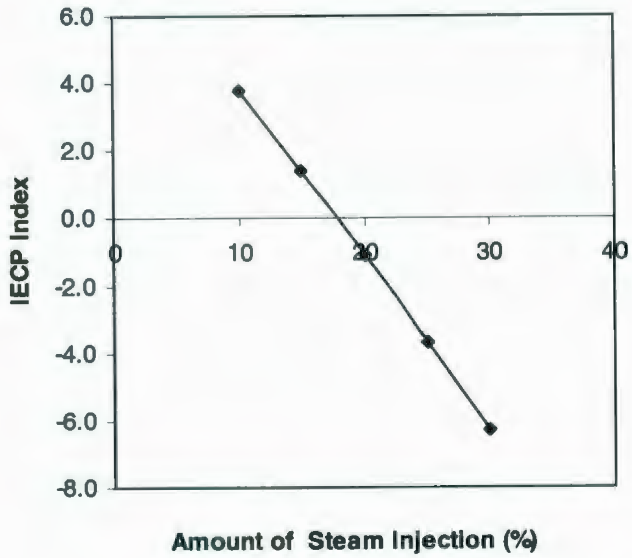

Figure 5.8: IECP Index for Different Steam Injection Options

i.e. 10 and 15% steam injection, have better performance than the base case. The maximum index value was obtained for 10% steam injection case. It is observed that like FGR, for both the water and steam injection cases, the value of IECP index becomes lower as the amount of injection increases. In case of water injection, water becomes evaporated upon injection, which takes a huge amount of latent heat and thus the net power output decreases (Schreiber, 1991). Like FGR case, this increases cost and CO_2 emission per unit power output and ultimately causes the lower IECP index.

In case of steam injection, the efficiency penalty is less as compared to the water injection case which causes the steam injection options to have higher index values.

For further screening of all the investigated options the value of Y was considered as 2, which ultimately selected only two options, i.e. 10% FGR and SI. The IECP indices for these options are 3.4 and 3.8 respectively, indicating 10% steam injection is the best option. However, both options might be selected for the further flowsheet development.

7.0 Conclusions

The proposed IECP approach has been successfully implemented in the Aspen HYSYS process simulator which provides an intelligent support to the designers for quick screening, evaluation and final selection of design alternatives.

In this paper, IECP approach has been applied to investigate different NOx prevention alternatives at the preliminary design phase of a 125 MW combined cycle power plant. Initially, the Aspen HYSYS tool generated a large number of design alternatives for NOx prevention by flue gas recirculation, water and steam injection to the furnace. The integrated use of IECP tool with the Aspen HYSYS, at first screens out the options that do not fulfill the NOx emission target, subsequently the selected options are evaluated in terms of environmental and economic aspects. Finally, only the options with higher potential are selected based on a predefined IECP index value.

Through the case study, the applicability of the IECP tool has been demonstrated. The results of the evaluation of different NOx reduction options are consistent with the findings of the previous researchers (Touchton, 1985; Weibel, 1993; US EPA, 1992), which demonstrate the robustness of the IECP tool.

The IECP tool is applicable to a wide variety of processes. Although in present case study, it has been successfully applied to investigate NOx reduction alternatives in a thermal power plant; more case studies need to be carried out to examine its wider applicability.

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Chapter 6

E-Green - A Robust Risk-based Environmental Assessment Tool for Process Industries

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Preface

This chapter presents a manuscript which describes a risk-based environmental assessment approach (E-Green) for evaluating different flowsheets at the preliminary design or retrofit stage. A version of this manuscript has been published in the journal of *Industrial Engineering and Chemistry Research* (Hossain et al., 2007).

The first author (Khandoker Hossain) participated in problems identification and formulation, and design of E-Green approach. Furthermore, he was also involved in the case study design and execution, analysis and interpretation of the results as well as writing the manuscript.

The co-authors (Drs. Khan and Hawboldt) supervised the development of work, reviewed the developed approach and case study results. They also critically reviewed the manuscript and provided valuable suggestions.

Abstract

This paper proposes a risk-based environmental assessment approach (E-Green) for evaluating different process options at early design or retrofit stage. The approach splits the cradle-to-gate life cycle into two domains: the raw materials production and supply domain and the process domain or gate-to-gate domain. It allows an analyst to investigate adverse impacts of the process activity on each domain separately and results in a more manageable assessment of process design alternatives. It is a risk-based approach contrary to the existing hazard-based approaches.

E-Green replaces the conventional normalization step of the impact assessment phase of a life cycle assessment (LCA) with a ranking step, which compares the effect scores of all the impact categories for different options and gives a relative score to each option. This eliminates the complexity and bias of the conventional normalization step in evaluation phase and enables the analyst to perform the effective evaluation easily. The applicability of the E-Green has been illustrated in the assessment of two solvent options in an acrylic acid manufacturing plant. E-Green methodology is implemented by combining Aspen HYSYS process simulator and a quantitative exposure assessment tool (E-Fast).

Keywords: Environmental assessment, Risk-based design, Process simulator, Pollution prevention

1.0 Introduction

Process industries and associated activities are major sources of emissions of harmful contaminants to the environment, which increase human and environmental health risks. Therefore, it is crucial to assess the process from an environmental perspective at design as well retrofit stages. Success of pollution prevention measures depends on the use of proper environmental assessment techniques. Life cycle assessment (LCA) is a useful tool for the systematic evaluation of environmental aspects of a product, service or process alternatives through all stages of its life cycle. LCA provides adequate means for environmental decision support and thus a significant effort has been devoted to develop environmental assessment tools based on LCA for environmental friendly product and process design (Steen, 1999; Goedkoop et al., 1995; Goedkoop and Spriensma, 2001; Cabezas et al., 1997).

For process evaluation two types of LCA approaches are commonly practiced in industries. In one approach, the environmental assessment is carried out over the cradle-to-gate life cycle, where toxic releases, materials' and energy consumptions at different stages of the life cycle are quantified. This includes the extraction, processing and transportation of raw materials, manufacturing, and final disposal (Gabel, 2001; Sadiq et al., 2005). In the second approach, the environmental burden of the process design or retrofit activities is quantified over the gate-to-gate life cycle i.e. within the boundary of the target industry (Cabezas et al., 1997; Cabezas et al., 1999; Young and Cabezas, 1999; Cardona et al., 2004).

Both types of the LCA approaches have certain limitations. In the gate-to-gate approach, the environmental impacts of the process activity are not considered over global system boundary, hence, the selected option based on this approach may have a less harmful impact on the local environment but significant impact on the global environment (Azapagic, 1999; Vyzi and Azapagic, 1998; Yates, 1998). In contrast, the cradle-to-grave or cradle-to-gate life cycle approach gives the same weight to the emissions of the target process and other emissions generated in different steps over the raw materials production and supply domain. However, the emissions of the target process generally have more direct impact on occupational health and safety, local population health as well as local ecological health, which should be given extra emphasis. It is likely that the option prioritized based on this approach has minimum impacts on the global environment but significant impacts on the local environment.

Most of the earlier efforts including WAR algorithm, used hazard-based approach to evaluate the environmental performance of different process options (Young et al., 1999; Brentrup et al., 2003). For each chemical, a toxicity indicator or toxicity potential is assigned, which indicates how much a particular chemical is toxic relative to a reference chemical or large number of chemicals (Young et al., 1999). Subsequently an overall toxicity index is calculated due to all releases associated with a process (Brentrup et al., 2003; Solnes, 2003). If the overall toxicity index of an option is lower relative to other options, then the option gets higher priority. This hazard-based evaluation can roughly indicate which option is relatively more environmental friendly, however it ignores the site-specific parameters of the process and its surroundings. As for example site specific parameters incorporate the ventilation system of the industry, average concentration in different area of the industry, the length of the time workers are exposed to a specific chemical, distance of the nearest population, consideration of sensitive people, wind data, and exposure routes. Therefore, it cannot be the ultimate decision making tool to set up a new industry or implement a retrofit option especially when the proposed/existing industry is located in a populated area. In contrast, the risk-based approach is more pragmatic as it takes account of site-specific parameters along with the likelihood of exposure. This facilitates one for realistic and effective decision-making in diverse scenarios.

In earlier efforts, different environmental options are compared based on an overall single toxic indicator, which is obtained by adding the weighted normalized indicators of different impact categories. However, in some cases significant difference in the normalized indicators may occur among different major impact categories. This may cause the overall toxic indicator to be biased by the impact category that has high value of normalized score (Brentrup et al., 2003).

This paper proposes a robust environmental assessment methodology (E-Green) to address the limitations of previous methods, which have the following features:

i. The methodology has split the cradle-to-gate system boundary into two domains: raw materials production and supply domain and gate-to-gate domain. Environmental assessment is conducted separately in each domain.

ii. Separate weighting factors are used for a particular impact category in each domain to give a different scale of emphasis to the category across the domains.

iii. In the impact assessment phase, the conventional way of normalization step has been replaced by a ranking step to make the decision-making process straightforward and robust.

iv. A quantitative risk-based approach is used for effect characterization.

v. Finally, the proposed approach includes the workers occupational health and safety category during the environmental assessment in the gate-to-gate domain.

The applicability of the E-Green approach has been demonstrated in an acrylic acid manufacturing process by evaluating the environmental performance of two solvent options.

2.0 Description of E-Green Methodology

The architecture of E-Green methodology is shown in Figure 6.1. The methodology is applicable at early design stage when designers evaluate different process options. It is equally applicable to any retrofit work of an existing process system. The methodology comprises two major steps: i) an inventory analysis, and ii) impact assessment, which are briefly discussed below.

2.1 Inventory Analysis

Inventory analysis involves the quantification of environmental burdens over the entire life cycle of a process or activity (ISO, 1998). Environmental burden accounts for any releases of contaminants that have potential adverse impacts on environment. It also considers the energy usage at different steps of the life cycle, where energy is not produced inside the process boundary. In the proposed methodology, the inventory analysis over the entire life cycle is split into two domains: i) inventory analysis over raw materials production and supply domain and ii) inventory analysis within the manufacturing premises. Analysis in the first domain considers all important hazardous releases and energy used due to raw materials extraction, manufacture, distribution, and all intervening transportation steps until the plant gate. In the second domain, inventory analysis estimates all the fugitive emissions during raw materials and product handling and manufacturing operations, energy consumption and the amount of hazardous chemicals released to air, water and soil. Fugitive emissions inside the premises help to determine the occupational health risk to the workers.

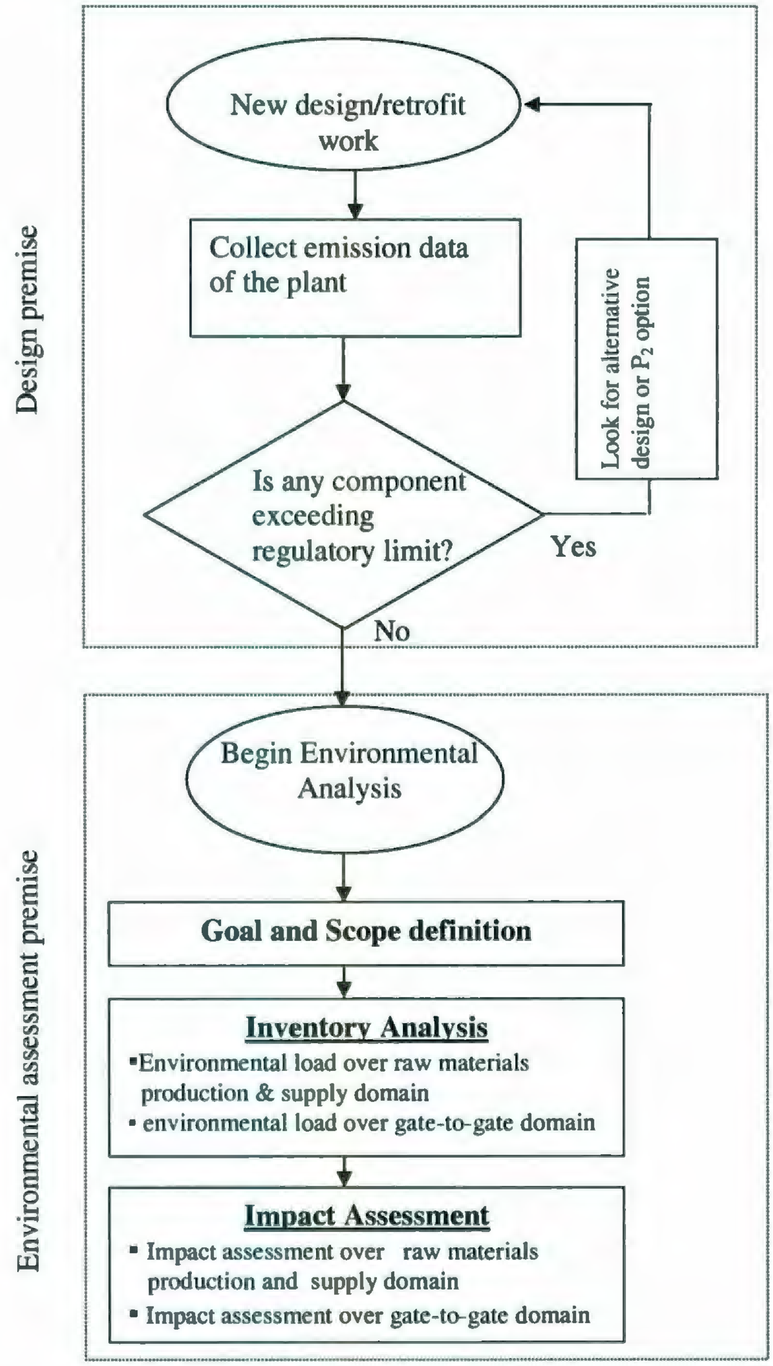

Figure 6.1: Schematic Representation of the Proposed Environmental Assessment Approach (E-Green)

2.2 Impact Assessment

The inventory data is very difficult to compare and interpret, therefore, ISO framework for LCA considers impact assessment to be an essential part of life cycle analysis followed by the inventory analysis phase (ISO, 14040). It consists of three steps: i) classification and characterization, ii) normalization, and iii) evaluation. Figure 6.2 shows different steps of the impact assessment. The steps are briefly discussed below.

2.2.1 Classification and Characterization

In classification step, all the inventory data is classified in to different classes according to their effects. For instance, classification of the emissions to air, water and soil, sorting of the air pollutants in accordance with global warming, ozone layer depletion, etc. In this characterization step, most of the earlier research has used the effects of the emissions over global, continental or regional boundary (Goedkoop et al., 2004), however, local impacts surrounding the industry are not considered. In proposed methodology, in gate-to-gate domain local impacts due to all significant industrial emissions are calculated, which will insure the environmental friendly process design. In order to characterise the effects of different emissions over the raw materials production and supply domain, only criteria air pollutants and their global impacts like global warming, ozone layer depletion and acid rain are considered.

For characterizing the effects, most of the early impact assessment approaches reported in the literature used hazard-based approach (Goedkoop and Spriensma, 2001).

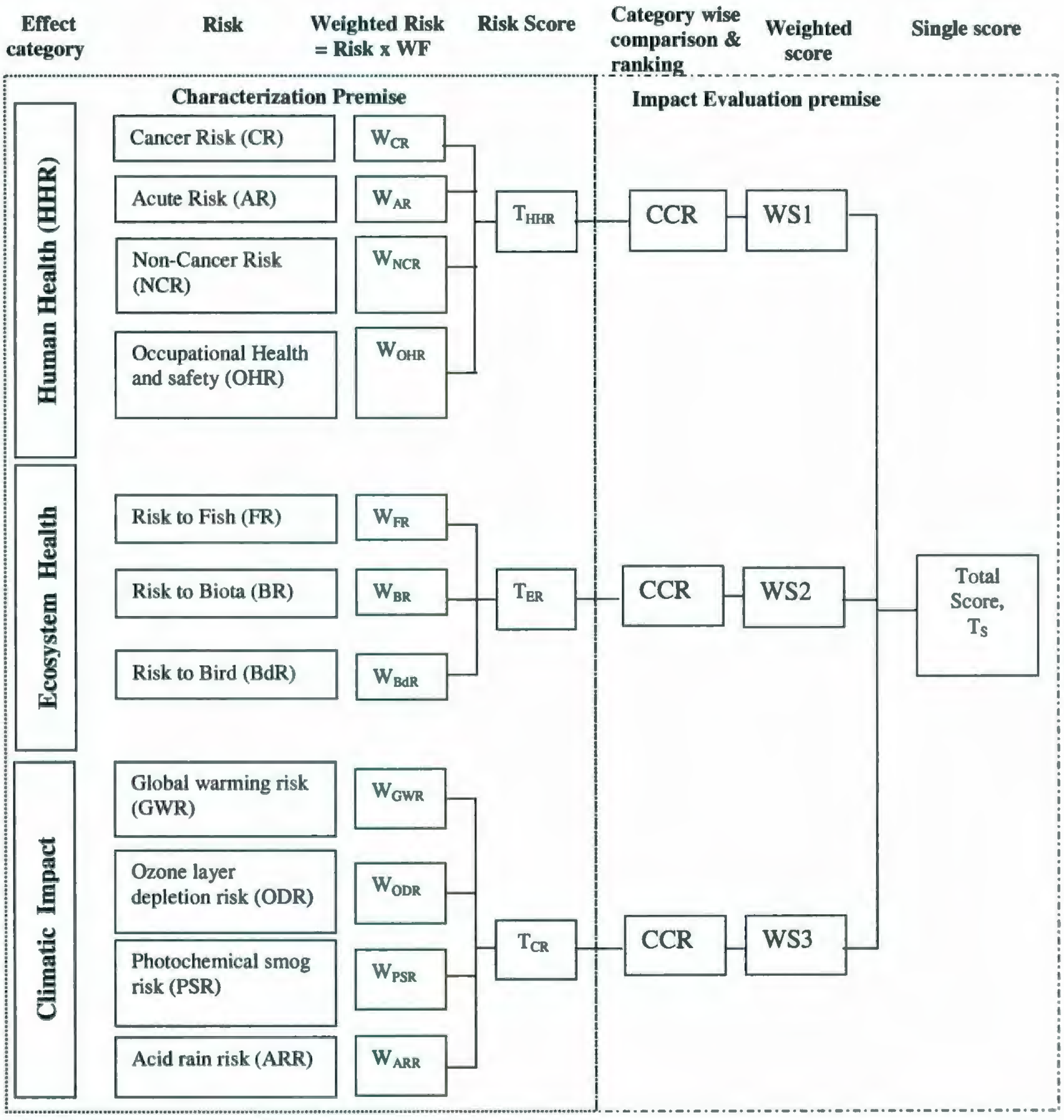

Figure 6.2: Different Steps of Impact Assessment in E-Green Approach

In present work, risk-based approach is used instead of hazard-based approach is used instead of hazard-based approach, where risks of different emissions are calculated for each effect category. Risk is considered as hazard with its probability of occurrence (LaGrega et al., 2001). For risk calculations the dose received by the concerned receptors are crucial to be considered. To estimate the dose, the use of exposure assessment tool could make the process faster. A number of exposure assessment tools are developed by the US EPA such as SRD, UCSS, ChemSTEER, GEMS and E-FAST. One can select any of them based on the requirements. Therefore, it gives more realistic picture over hazard for decision-making. Inclusion of the number of effect categories/subcategories in the risk assessment is subject to a number of factors such as the release scenarios, location of the industry, population destination, etc. For instance, if an industry is located in a remote area then risk assessment to human health is not considered important in gate-to-gate domain. Though Figure 6.2 has included most of the impact categories, however, the decision of the inclusion of impact categories depends on the evaluators.

2.2.1.1 Algorithms for Risk Characterization

The following algorithms provide guidelines on how to quantify risk in both domains of the life cycle. The total risk of a process option to a particular impact category *k* over a cradle-to-gate domain is equal to the total risk to an impact category *k* due to the emissions over raw materials production and supply domain plus the risk to *k* impact category due to the emissions over gate-to-gate domain. This may be mathematically represented as:

$$R_{tot\,cat-k} = R_{LCA\,raw\,cat-k} + R_{pros\,cat-k} \tag{6.1}$$

If the energy generating unit is located inside the plant boundary then its environmental load can be seen in gate-to-gate inventory analysis, however, if it exists outside the plant boundary i.e. energy consumed is supplied from grid, then its environmental effect can not be seen. In this situation the total risk due to the concerned process plant includes risk due to the production of energy consumed in the plant operation. Therefore, equation (6.1) becomes:

$$R_{tot\,cat-k} = R_{LCA\,raw\,cat-k} + R_{pros\,cat-k} + R_{pros\,energy\,cat-k} \tag{6.2}$$

2.2.1.2 Risk Characterization over Raw Materials Production and Supply Domain

To estimate risk in this domain, one needs to consider all releases from natural resources extraction, intermediate processes for raw materials production and raw materials supply to the target process input gate. This mainly involves three types of emissions: emissions generated in the process operations, emissions associated with the energy production consumed by different process operations, and the emissions associated with the transportation steps. If $R_{m\ Cat\text{-}k}$ denotes the risk to an impact category *k*, due to the total emissions over a raw material's production and supply domain then,

$$R_{m\,cat-k} = \sum_{q=1}^{p} \psi_{t,k,q} + \sum_{s=1}^{z} \psi_{e,k,s} + \sum_{s=1}^{z} \sum_{j=1}^{n} \sum_{c=1}^{x} \psi_{c,j,s,k} \qquad (6.3)$$

Where, s is the number of intermediate production steps to produce a raw material m, j is the number of waste streams, $\psi_{c,j,s,k}$ is the risk of a component c to an impact category k for a stream j of a production step s. $\psi_{e,k,s}$ is the risk to an impact category k due to the emissions associated with the energy production consumed by the process in a production step s. $\psi_{t,k,q}$ is the risk to category k due to the emissions of a transportation step q. So, total risk for all the associated raw materials to a category k is:

$$R_{LCAraw\,cat-k} = \sum_{m=1}^{n} R_{m,cat-k} \qquad (6.4)$$

2.2.1.3 Risk Characterization Over Gate-to-gate Domain

In the gate-to-gate domain two types of material streams are considered: input material streams and outgoing material streams. In addition, if energy is not generated inside the boundary of the plant then total energy consumed by the process, utility systems and other supporting systems also need to be considered because in such case the effect of energy use will not be seen in input and output streams. If $R_{in\ Cat-k}$ is the risk due to the handling of all input materials to an impact category k then:

$$R_{in\ cat-k} = \sum_{i=1}^{n} \psi_{i,k} \tag{6.5}$$

Where, i is the number of input materials, $\psi_{i,k}$ is the risk to an impact category for handling the input materials to impact category k. Therefore, for different impact categories equation (6.5) may be used repeatedly. The handling of input materials has a greater contribution to occupational exposure and therefore, workers health and safety. For outgoing streams, risk is estimated using the following equation:

$$R_{out\ cat-k} = \sum_{j=1}^{m} \psi_{c,j,k} + \sum_{p=1}^{z} \psi_{p,k} \tag{6.5a}$$

Where, j denotes the number of waste streams, c is the number of components in a stream j. $\psi_{c,j,k}$ is the risk to category k due to the release of component c in stream j. $\psi_{p,k}$ is the risk for workers exposure due to handling of single or multiple products. Therefore, risk over the gate-to-gate domain for a particular impact category k is:

$$R_{pros\ cat-k} = R_{in\ cat-k} + R_{out\ cat-k} \tag{6.6}$$

It is important to note that unless the product life cycle is considered, the product has very little impacts on environmental health, however, has considerable impact on workers occupational health and safety. Therefore, in equation 6.5(a), the second term is only considered when risk of the outgoing streams is calculated over the occupational health and safety category. As risk cannot be correlated accurately with per unit mass of the product, in the above equations the risk within the process boundary needs to be calculated based on the total emissions due to the product and raw materials flow rate. Over different steps of the raw materials production and supply domain the emissions calculation is based on the required amount of input raw materials flow rate.

Using equations 6.1 and 6.2, one may estimate risk over the cradle-to-gate boundary to a particular impact category. Similar procedure may be repeated for estimating risk over other categories.

2.2.2 Ranking

In E-Green approach, ranking has replaced the conventional normalization step. Normalization is usually used to compare the calculated effect scores on a common scale in order to get better understanding of the relative size of an effect. Normalization results in a set of effect scores, which have the same or no dimension and reduce the difference among different categories data (Goedkoop and Spriensma, 2001). It is done using some reference values; a commonly used reference value is the average environmental load per year of an inhabitant in a specific country or region (Goedkoop et al., 2004). Although normalization compares all the impact categories on a same scale, it does not say anything about the relative importance of different impact categories. Therefore, normalization results cannot be used for final judgement. Usually, normalized scores of each category are multiplied by a weighting factor, which are subsequently added to get an overall single score.

As normalized scores greatly depend on the reference value, therefore, result is likely to vary between two analysts due to the use of different reference values. It is difficult to take decision about which reference value should be used. Besides, in different countries or regions there is a lack of reliable environmental data for reference values. Sometimes, a significant difference may exist between the normalized scores, especially when the nature of the two data categories is quite different due to the different reference values for different data categories (Brentrup et al., 2004), in such situation assigning of weighting factors may not produce reliable result because the overall single score has greater chance to be biased by the impact category having higher normalized risk score. It is worth mentioning that in risk-based approach such differences in normalized scores are more common compared to the hazard based approach.

In order to address the problems with normalization, in the proposed impact assessment approach, the conventional normalization step is replaced by a ranking step (Figure 6.2). The ranking step compares risk scores of a specific effect category for different options and based on the comparison, different scores are applied to the options. The risk score of different options for a particular category k is divided by the average risk score in order to assign a ranked score to each option. For instance, risk scores for human health category of five investigated options are 50, 40, 30, 25 and 10. Therefore, calculated ranked score for the options will be 1.61, 1.29, 0.9677, 0.806, and 0.3225 respectively (Figure 6.3).

As compared to the conventional normalization approach, the proposed ranking approach is very simple, provides consistent results among different analysts, and eliminates the difficulty of selecting the reference values. In addition, for a particular impact category the difference between the ranked scores is usually within a narrow range. Thus, for a particular option, the difference among different impact categories is also likely to be insignificant, which would significantly reduce the bias on the decision-making unlike the conventional normalization procedure.

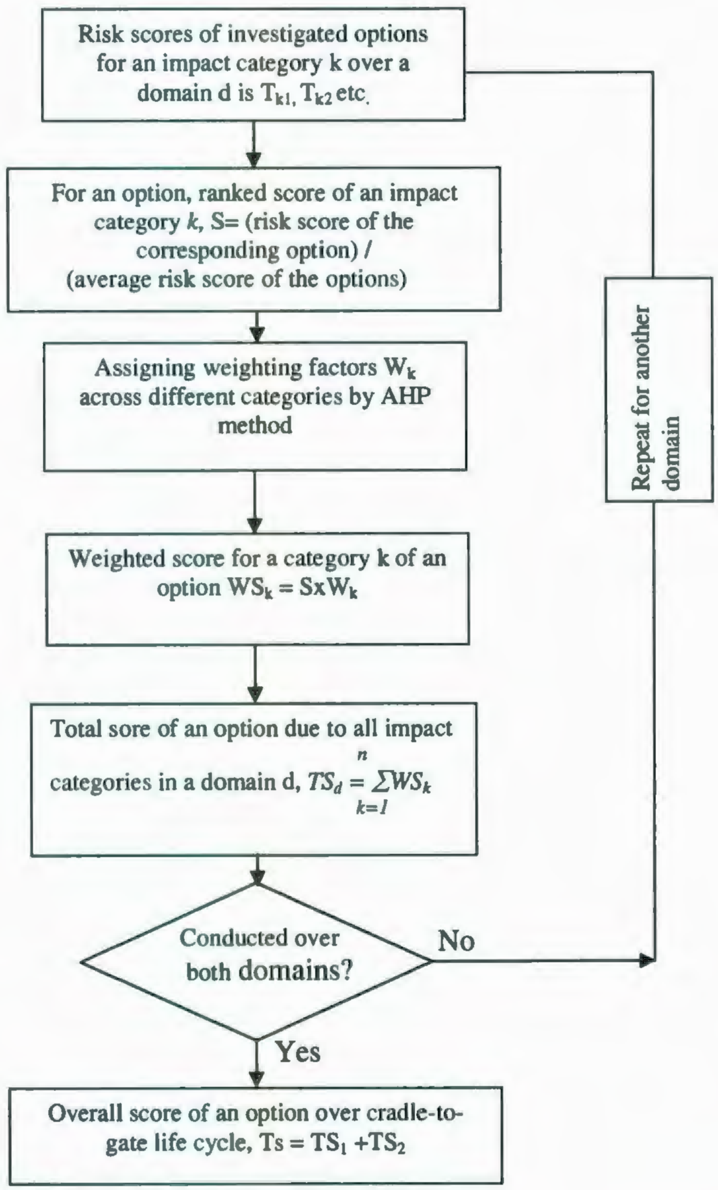

Figure 6.3: Different Steps of the Proposed Ranking and Evaluation Approach

2.2.3 Evaluation

Although ranking can provide a set of scores for a particular option, yet, it cannot be used to interpret the result. Like normalization, it does not say anything about the relative importance of different impact categories. To resolve this problem, ranked scores of different impact categories are multiplied by weighting factors, which are subsequently added to obtain an overall single score (Figures 6.2 and 6.3). According to the ISO 14042, weighting is an optional step of a life cycle impact assessment.[18] Some LCA methods have not used the weighting step (IPCC 2001; CMLCA, 2004), while others have (Goedkoop et al., 1995; Goedkoop and Spriensma, 2001; Steen, 1999; Wenzel et al., 1997). The weighting step can be eliminated for the cases when the normalized/ranked scores of an option are always higher over other options or the assessment considers only one impact category (Goedkoop and Spriensma, 2001). It can also be dropped when the assessment aims to determine the total environmental burden over the entire life cycle.

Weighting is the most controversial step of the impact assessment (Goedkoop and Spriensma, 2001). Weighting factors have been determined in the literature based on any of the following principles: cost of health care, pollution preventing cost, the evaluation of experts, gap between the current impact level and target level, actual damage or analytical hierarchy of the impact categories (Goedkoop et al., 1995). In proposed methodology, an analytical hierarchy process is used (Saaty, 1980; Slones, 2003).

Figure 6.3 shows how ranked scores are converted to an overall single score using the weighting factors. Weighting factors for a specific impact category across two domains may differ, which will provide a different degree of emphasis to a particular category across the domains. However, the earlier cradle-to-gate or cradle-to-grave

LCA has not considered the local impacts due to the process emissions differently i.e. same weight has been given to a particular impact category throughout the life cycle. If the weighting factor is same for both domains, the assessor has given the same importance to both local and global impacts, which may not lead to an environmentally benign and sustainable option from local environmental perspectives.

3.0 Application of E-Green

The applicability of the E-Green has been illustrated in the assessment of two solvent alternatives in an acrylic acid manufacturing plant. The E-Green methodology is implemented by combining Aspen HYSYS process simulator and a quantitative exposure assessment tool, E-Fast.

3.1 Process Description

A schematic representation of acrylic acid manufacturing process is shown in Figure 6.4. The process is designed to produce about 50,000 T/year of acrylic acid with purity above 99.9% (Turton et al., 2003). Compressed air, propene and steam are fed to a reactor where acrylic acid and some acetic acid are formed through the following catalytic reactions. The reactor temperature is kept constant at 310 °C.

$$C_3H_6 + 3/2\,O_2 \longrightarrow C_3H_4O_2 + H_2O$$

$$C_3H_6 + 5/2\,O_2 \longrightarrow C_2H_4O_2 + H_2O + CO_2$$

$$C_3H_6 + 9/2\,O_2 \longrightarrow 3H_2O + 3CO_2$$

After the reaction, product is sent to a flash tank where it is rapidly quenched to avoid further oxidation reactions. The quenching is achieved by injecting a recycled stream of aqueous acids. The bottom product mixture from the flash chamber consists of acetic acid and acrylic acid. The vapour is sent to an absorber column where additional recovery of the liquid acid mixture is achieved. The off-gas from the absorber is released to the air.

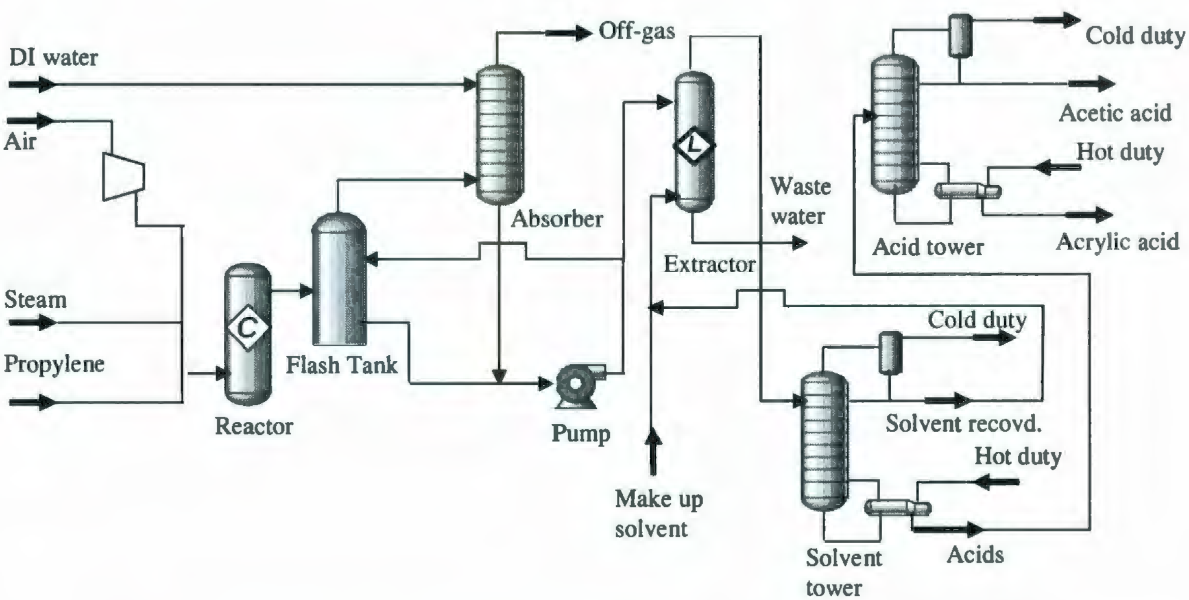

Figure 6.4: Schematic Representation of Acrylic acid Production Process

The dilute acid stream from the absorber is mixed with the bottom acids stream of the flash tank and a portion of final stream is recycled to flash tank as quenching medium. Due to the high cost of water distillation, a solvent is used to extract the water from the aqueous acids mixture. A range of solvents could be used for water extraction, of which some common are diisopropyl ether, ethyl acetate, xylene, diisobutyl ketone, methyl isobutyl ketone and ethyl acrylate (Turton et al., 2003). The aqueous acids are sent to an extraction column where the acids are extracted from water using the solvent. The water is discharged as wastewater and contains trace amounts of solvent. The solvent is recovered from the acid solvent mixture in a solvent tower. The solvent is recycled back to the extraction tower. The acid mixture is sent to an acid distillation tower where acrylic acid is separated as bottom product and acetic acid as top product. The purity of acrylic acid and acetic acids are above 99.9% and 95% respectively.

The objective of this case study is to investigate the environmental performance of isopropyl acetate compared to a common solvent ethyl acetate. In order to get detailed process data for both options, the acrylic acid manufacturing process is simulated for the both cases using Aspen HYSYS process simulator.

3.2 Inventory Analysis, Risk Characterization and Impact Assessment

Table 6.1 shows the input materials and waste flows of the acrylic acid plant for the two options. In waste stream only trace components are shown. The energy is delivered to the plant from grid and, therefore, no emission due to energy generation is shown in Table 6.1. However, the equivalent amount of emissions due to energy consumed needs to be considered over the raw materials production and supply domain. For life cycle inventory assessment of raw materials, all the intermediate production steps starting from the natural sources are considered. Figure 6.5 shows the production chains for ethyl acetate and isopropyl acetate considered in this study. To calculate the total environmental burdens over raw materials production and supply domain, energy consumed in process and transportation, and important

Table 6.1: Input and Waste Flows of Acrylic Acid Plant

	Option 1 (Base case)	**Option 2** (Alternative case)
Input materials kg/h		
Propylene	5,344	5,344
Steam	17,880 38,528	17,880 38,528
Air	44,053	
Ethyl acetate		61,280
Isopropyl acetate		
Off-gas composition, kg/hr (mass flow)		
Propene	7,12.9	712.9
CO_2	2,595.2	2,595.2
Waste water composition		
Mass flow, kg/hr		
Ethyl acetate	2012	
Isopropyl acetate		556.61
Acetic acid	12.65	2.08

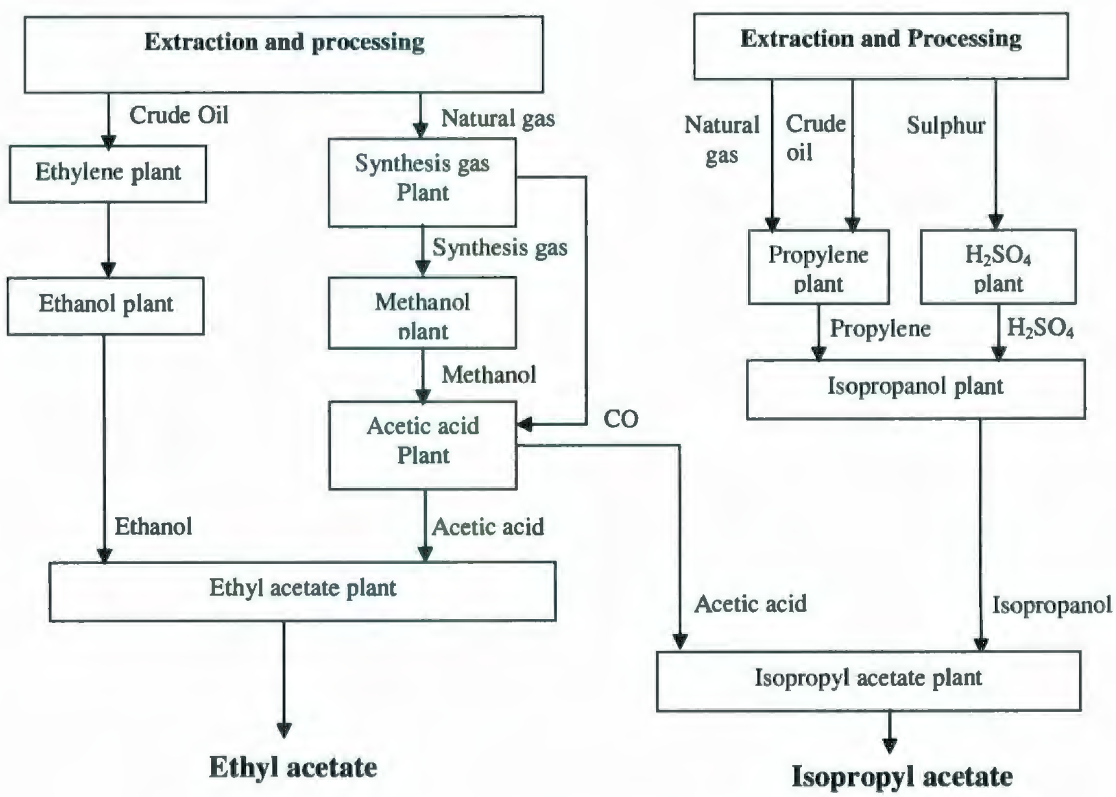

Figure 6.5: Production Chain for Ethyl Acetate and Isopropyl Acetate

hazardous releases in each production step are taken into account. The significant emissions of the two solvents over each domain due to energy used, manufacturing and other activities are shown in Table 6.2, which are calculated with the help of eco-invent life cycle database (Ecoinvent, 2006).

Table 6.2: Life Cycle Emissions Data for Two Solvents (for 1 kg)

Contaminants	Option 1		Option 2	
	Gate-to-gate domain kg	Raw material domain kg	Gate-to-gate domain kg	Raw material domain kg
CO_2	0.058	1.5682	0.042	1.6512
CO	-	0.0054	-	0.0046
SO_2	-	0.0060	-	0.0065
NO_x	-	0.0055	-	0.0056

Exposure assessment has been conducted using the US EPA EFAST V2.0 software. E-FAST V2.0 is a tool for potential exposure assessment from chemical discharges to air (stack or fugitive releases), surface water, or land. In addition, E-FAST also can be used to assess inhalation and dermal exposures to chemicals that result from the use of certain types of consumer products. It employs different multimedia fate and transport models to estimate potential exposures through different exposure routes and pathways. The exposure scenarios in E-FAST V2.0 contain default exposure parameter values that allow for estimating the exposures with minimal data entry (E-FAST, 2006).

In this case study, the nearest population considered is 500 meters far from the plant. As risk assessment is scenario specific, risk assessment values calculated for unit product or unit amount of contaminants release could not be used as a basis because multimedia fate and transport model for exposure assessment is usually non-linear in nature. Therefore, the generalized exposure assessment concept based on a unit amount of a chemical's release is questionable and may not produce reliable results (Herthwich et al., 2000; Goedkoop et al., 1995; Goedkoop and Spriensma, 2001). The total production rate for both process options is considered the same to compare the risk assessment values from two process options. Aspen HYSYS is used to generate data at a same production rate for the two process options. With the aid of the E-FAST software, human carcinogenic dose, non-carcinogenic dose and acute concentrations of the chemicals released for different routes are calculated. The software is also used to determine the chemical concentration in the water body receiving the wastewater for ecological risk assessment. For work place exposure assessment, the concentration of contaminants in the air is calculated from fugitive emissions from different possible sources. Another way to estimate the concentration in the work place air is by sampling over a specific period of time for a particular scenario. In this paper, the time-weighted average of work place concentration in the air is considered. Workers' carcinogenic and non-carcinogenic risks are calculated considering eight hours a day, five days a week and thirty-year exposure duration using the following equations:

$$\text{Cancer Risk} = I_c \times SF \quad (6.7)$$

Where, I_c = chronic daily intake of carcinogen (mg/kg.day)

SF = carcinogen slope factor (kg.day)/mg

$$\text{Non-Cancer Risk} = HI = I_N / Rfc \quad (6.8)$$

Where, HI = hazard index

I_N = chronic daily intake of non-carcinogen (mg/kg.day)

Rfc = reference concentration

For estimating climatic risk for a particular category, environmental indicator from the EPI database has been used to obtain the potential effect per unit mass (EPI, 2001). This value is multiplied by the total release of the chemical to determine the total hazard to a specific effect category due to the emission. The obtained hazard value is subsequently multiplied by the likelihood of occurrence in order to obtain the risk to a specific climatic effect category.

For determining the weighting factors WS1, WS2 and WS3 opinions from different people working in this area risk are collected which is analyzed using analytical hierarchy method. The values of WS1, WS2 and WS3 are determined as 2, 1and 1 respectively.

The overall score for a particular option over the investigated life cycle is calculated using the method shown in Figure 6.2. In order to compare the results obtained in a risk-based approach with those of hazard-based approach, the same case study has been conducted by applying E-Green based on a hazard based effect characterization approach.

4.0 Results and Discussions

Figure 6.6 shows the ranked score of the two investigated options for human health category over the gate-to-gate life cycle domain. It is observed that the isopropyl acetate option has less score compared to the ethyl acetate option, which indicates that the isopropyl option is less detrimental to human health. Figure 6.7 shows the comparison of the two options in gate-to-gate domain in terms of ecological impact. From the figure it is apparent that the isopropyl acetate option has less impact on ecological health than the ethyl acetate option due to its lower score.

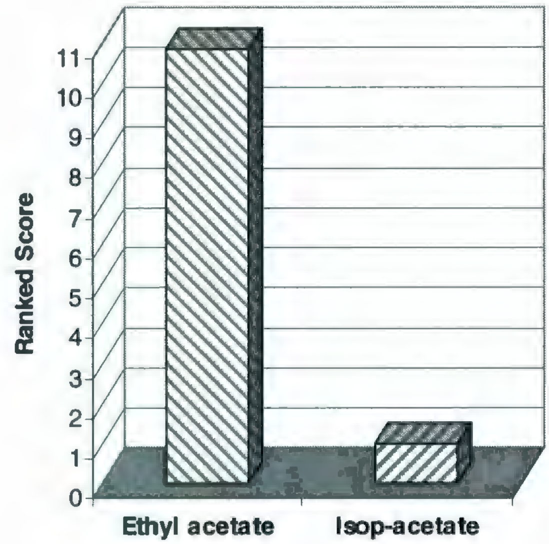

Figure 6.6: Human Health Ranked Score for Both Options Over Gate-to-Gate Domain.

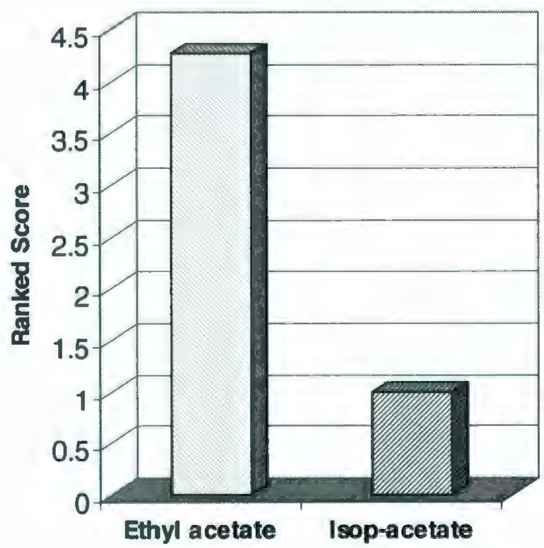

Figure 6.7: Ecological Health Ranked Score for Both Options Over Gate-to-Gate Domain.

The climatic effect for the two options over the gate-to-gate domain is presented in Figure 6.8. It shows that the both options have equal climatic impact score. This is due to the fact that production rate and composition of the off-gas remains same for the both options (see figure 6.4) and the effect of energy on climate consumed within the process boundary is not considered over the gate-to-gate domain.

In Figure 6.9 climatic impact of two options over the raw materials production and supply domain is compared. It is observed that the isopropyl acetate option has higher value of ranked score in this domain, which indicates that the amount of total toxic contaminants released in the isopropyl acetate production and supply domain has higher overall risk to climate compared to that of the ethyl acetate option. From Figures 6.6 - 6.9, it is apparent that one option does not always result in better environmental performance as compared to the other option for all impact categories over both domains. The importance of different impact categories is not same for a

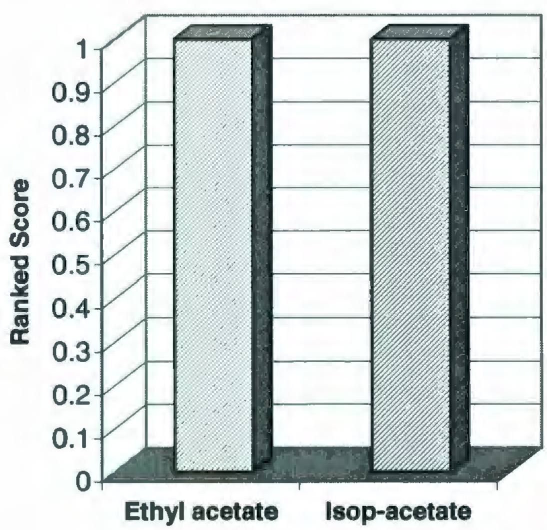

Figure 6.8: Climatic Impact Ranked Score for Both Options Over Gate-to-Gate Domain.

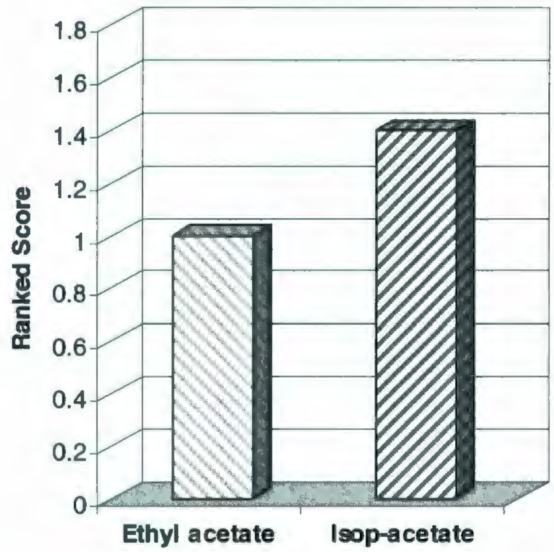

Figure 6.9: Climatic Impact Ranked Score for the Investigated Options Over Raw Materials Life Cycle Domain.

particular domain and it might also vary across the domain. Therefore, the option, which has a lower ranked score over more impact categories, is not necessarily the preferred option. It is very difficult for the analyst to take decision in this complex situation. The situation will increase in complexity as the number of option increases. To overcome this issue, all the ranked scores for a specific option over the cradle-to-gate domain are converted to an overall score by using weighting steps (Figures 6.2 and 6.3).

Figure 6.10 shows the overall ranked score of the two options over their cradle-to-gate life cycle domain. The figure shows that the isopropyl acetate option has lower overall ranked score than the ethyl acetate option, which indicates that the isopropyl acetate option is overall more environmental friendly considering both global and local impacts over the ethyl acetate option. According to the E-Green methodology, in the design phase it is ensured that only the options, which are not releasing any components beyond the regulatory level, will be assessed.

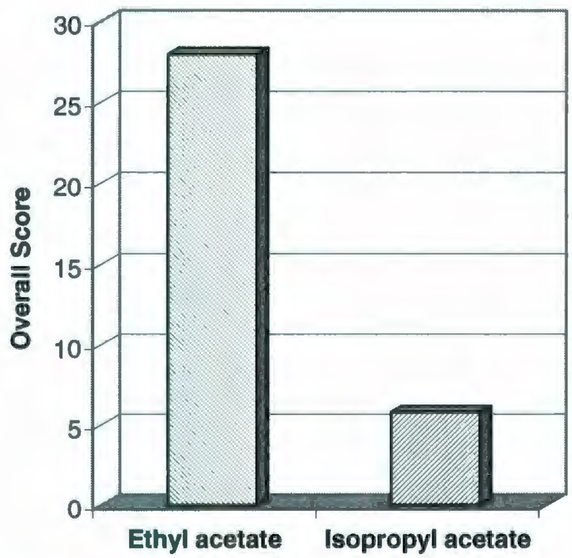

Figure 6.10: Overall Score for the Investigated Options Over Cradle-to-Gate-Domain.

Therefore, in this case both the options could be considered as environmentally friendly and should go through multi-criteria optimization and decision-making for identifying the overall better option considering economic, technical and other important criteria. However, as the isopropyl acetate option has better environmental performance, it will get more points during multi-criteria optimization and decision-making over the ethyl acetate option.

In above results E-Green uses risk based effect characterization, however, E-Green is also applicable for hazard-based effect characterization. The results obtained using hazard based effect characterization are shown in Figure 6.11– 6.15. Figures 6.11-6.14 represent the ranked score of the investigated options for different impact categories over the two domains and Figure 6.15 shows the overall single score over the cradle-to-gate domain. The comparisons of these results with risk-based results show that in all cases the results significantly differ between the two effect characterization approaches.

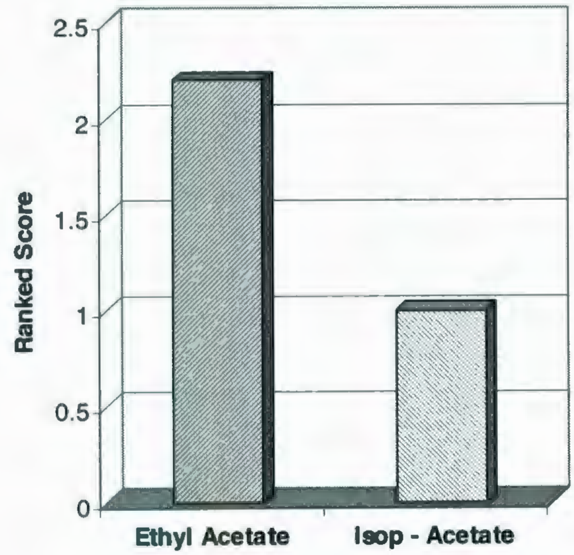

Figure 6.11: Human Health Ranked Score Obtained for Both Options Over Gate-to-Gate Domain Using Hazard-Based Approach.

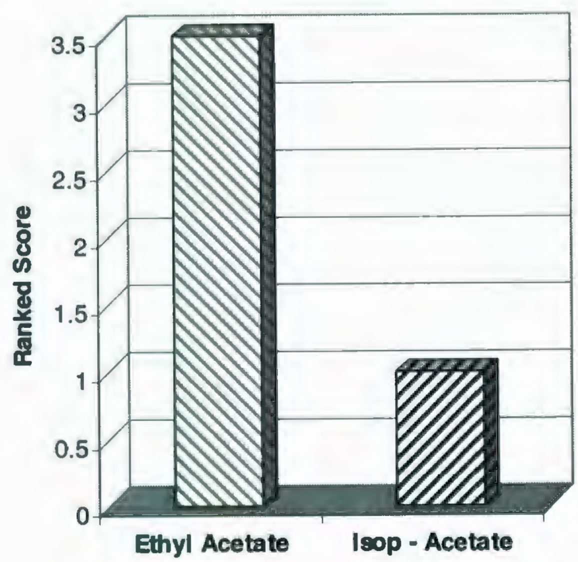

Figure 6.12: Ecological Health Ranked Score Obtained for Both Options Over Gate-to-Gate Domain Using Hazard-Based Approach.

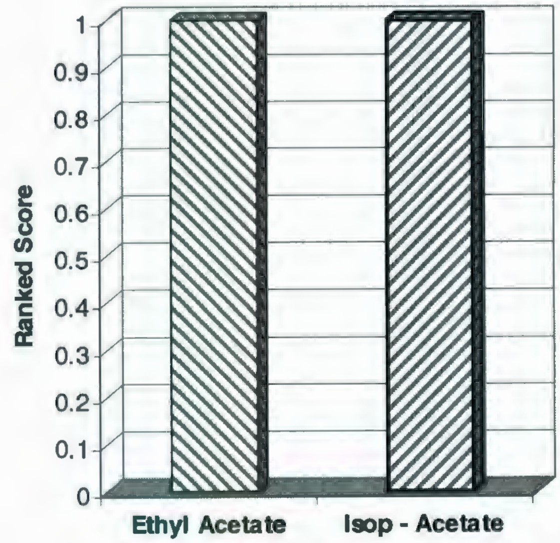

Figure 6.13: Climatic Impact Ranked Score Obtained for Both Options Over Gate-to-Gate Domain Using Hazard-Based Approach.

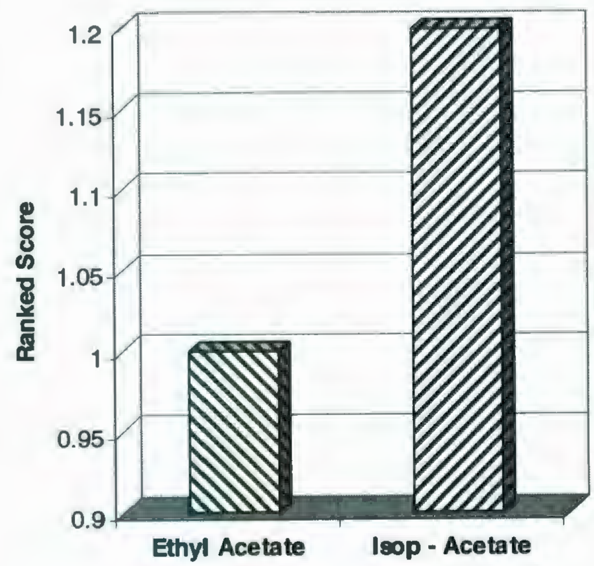

Figure 6.14: Climatic Impact Ranked Score Obtained for the Investigated Options Over Raw Materials Life Cycle Domain Using Hazard-Based Approach

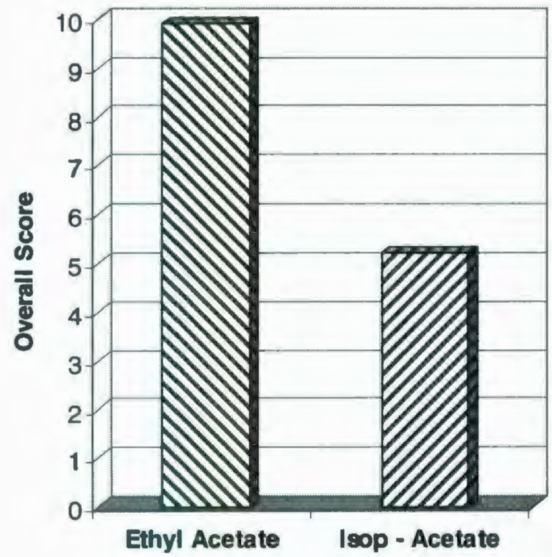

Figure 6.15: Overall Score Obtained for the Investigated Options Over Cradle-to-Gate Domain Using Hazard-Based Approach

In Figure 6.15 although hazard-based approach shows that the isopropyl acetate option is about two times better than the ethyl acetate option in terms of overall single score, the corresponding risk-based result (Figure 6.10) shows that isopropyl acetate option is about five times better. The difference in results between the two effect characterization approaches are due to the fact that hazard does not consider the site-specific parameters, therefore significant changes occur during multi-media fate and transport of the chemicals.

5.0 Conclusions

A general environmental assessment methodology (E-Green) for process designs and retrofit activities is presented. It has significantly modified the impact assessment phase of a conventional LCA. The methodology has been integrated with a process simulation tool Aspen HYSYS and an exposure assessment tool (E-fast) to enhance its robustness. It has following features:

i) It has split the cradle-to-gate life cycle assessment into two domains i.e. raw materials production and supply domain and gate-to-gate domain, which brings the opportunity to the analyst to classify, characterize and evaluate the impacts separately in two domains according to the needs. It would help to select the option, which is benign from both global and local environmental perspectives.

ii) It has eliminated the conventional normalization step and introduced a ranking step followed by the characterization step in the impact assessment phase. This attempt has been made to completely eliminate the potential biasing effect on the overall single score caused by the significant difference of the normalized scores across the effect categories. The ranking step is much easier and less time consuming, which would make the E-Green a robust environmental assessment tool for process industries.

iii) It has used risk-based effect characterization approach, which is more pragmatic over the conventional hazard based approach and therefore, enables the analyst to take more realistic and effective decision in diverse scenarios compared to the hazard-based approach.

The ranking approach is equally applicable for the cradle-to-grave LCA for assessing products or services. From the case study it has been realized that E-Green approach is easily applicable and less time consuming and it is also applicable for hazard-based effect characterization. The case study shows that the results obtained by the two effect characterization approaches are significantly different. E-Green is still at early stage of its application, however, it has introduced some important aspects of life cycle assessment based on which the further development could be continued. Research is ongoing to apply the E-Green in different real life case studies to check its robustness in diverse process scenarios.

6.0. Nomenclature

$R_{tot\ cat\text{-}k}$	Total risk to an impact category *k*
$R_{LCA\ raw\ cat\text{-}k}$	Risk to an impact category *k* due to the emissions over cradle-to-gate life cycle domain (i.e. raw materials production and supply domain)
$R_{pros\ cat\text{-}k}$	Risk to an impact category *k* due to the emissions over process gate-to-gate domain
$R_{pros\ energy\ cat\text{-}k}$	Risk to an impact category *k* due to the emissions concerned with the production of energy consumed in a process unit
$R_{m\ Cat\text{-}k}$	Risk to an impact category *k* due to the emissions related to the Production and supply of a raw material *m*
$R_{in\ Cat\text{-}k}$	Risk due to the handling of all input materials to an impact category *k*
$R_{out\ Cat\text{-}k}$	Risk to an impact category *k* due to all product and waste streams

$\psi_{c,j,s,k}$ Risk to an impact category *k* due to a component *c* of a waste stream j in a production step *s*

$\psi_{e,k,s}$ Risk to an impact category *k* due to the emissions associated with the production of the energy consumed in a production step *s*

$\psi_{t,k,q}$ Risk to an impact category *k* due to the emissions from a transportation step *q*

$\psi_{i,k}$ Risk for handling of an input material stream *i* to an impact category *k*

$\psi_{p,k}$ Risk to an impact category *k* due to a product stream *p*

$\psi_{c,j,k}$ Risk to an impact category *k* due to the release of a component *c* in a waste stream *j*

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Chapter 7

Conclusions, Novelties and Future Work

7.0 Conclusions

In the present work, an integrated approach for pollution prevention (P2) has been developed to facilitate the implementation of the P2 during process design and retrofit applications. It has the following attractive features:

- Risk and safety are incorporated as an additional objective function along with cost, technical feasibility and environment during the optimization of a design option.
- Multi-criteria optimization is used in the feasibility analysis phase, where different potential end-of-pipe options are considered along with the potential P2 alternatives.

These features make the IP2M approach robust for the sustainable design of process systems. To facilitate the generation of different P2 options, the present work has developed a process design approach (SusDesign). It helps in developing a number of optimal flowsheet designs by:

- Carrying out the analysis, evaluation and screening of the design alternatives at every level of process synthesis, which facilitates the screening out of inefficient options at the early stage of design.

- Incorporating environment as a design objective along with cost which facilitates the generation of sustainable process design.
- Carrying out quantitative evaluation of each design alternative, which will provide a strong basis for selecting the potential options.
- Integrating different thermodynamic tools to facilitate the generation, analysis, screening and optimization of design alternatives.
- Organizing designers' knowledge with the aid of a number of guidewords under the hierarchy of P2 strategies and some engineering tools.

The proposed SusDesign approach was demonstrated in the design of a 30 MW natural gas fired power plant and resulted in an efficient, cost effective and environmentally friendly system design. The final design achieved an overall thermal efficiency of 70%, CO_2 emissions of 0.28 kg/kWh and NOx emissions of 0.197 g/kWh, while in a typical natural gas fired power plant the thermal efficiency is about 35%, emissions of CO_2 and NOx are about 0.55 kg/kWh and 1g/kWh respectively. The case study shows that the application of SusDesign approach has improved the environmental and economic performance of the design gradually throughout different design stages. In the SusDesign, the alternative design options generated at preliminary process design are evaluated based on environmental and economic performance. At this stage, usually a huge number of options are required to be evaluated; therefore, a simple and quick quantitative evaluation approach is very crucial and to aid this, in the present work the IECP approach has been developed.

Using the IECP tool, the IECP index is calculated for each design option, which serves as the basis to evaluate the option from environmental and cost perspectives. The main feature of the IECP tool is that it could be easily integrated with a process simulation tool. This renders an intelligent support for the quick quantitative analysis, evaluation and selection of the design alternatives with most potential at each level of process synthesis. The IECP index also serves as a basis for the structural and parametric optimization of a flowsheet in terms of environment and cost. The IECP tool has been successfully applied to investigate different NOx prevention alternatives at the preliminary design phase of a 125 MW combined cycle power plant. Initially, the Aspen HYSYS has modeled a large number of design alternatives for NOx reduction by flue gas recirculation and water/steam injection. Through the application of IECP tool, only the optimal options are selected. The performance evaluation results of different options by the IECP tool are consistent with the findings of the previous researchers (Touchton, 1985; Weibel, 1993, US EPA, 1992), which demonstrate the robustness of the IECP tool.

One of the major steps of the IP2M approach is the detailed environmental evaluation of a group of P2 options or candidate flowsheets. For this, in the present work, a robust risk-based environmental evaluation approach (E-Green) has been developed, which has the following features:

- The cradle-to-gate life cycle assessment is split into two domains i.e. raw materials production and supply domain, and gate-to-gate domain. This facilitates the classification, characterization and evaluation of the impacts separately in each domain according to the needs. It helps selecting an option, which is benign from both global and local environmental perspectives.
- Elimination of the conventional normalization step and introduction of a ranking step in the impact assessment phase. This eliminates the potential biasing effect on the overall single score caused by the significant difference of the normalized

scores across the effect categories. The ranking step is much easier and less time consuming, which makes the E-Green a robust tool for carrying out the detailed environmental assessment of a process flowsheet.

- Risk-based effect characterization is used as it is more pragmatic over the conventional hazard-based characterization. This enables one to make more realistic and effective decision in diverse scenarios.

The applicability of the E-Green approach has been illustrated through the assessment of two different flowsheet options of an acrylic acid manufacturing plant. The E-Green approach has been implemented in combination with the Aspen HYSYS process simulator and a quantitative exposure assessment tool (E-Fast), which provides strong data and computational support to carry out the environmental assessment of the design options very quickly.

7.1 Novelties in the Present Work

Through the development of IP2M, SusDesign, IECP and E-Green approaches, the author has the following original contributions to the sustainable development of process systems:

- Development of an integrated pollution prevention approach which incorporates all the essential elements for the sustainable development of a process system.
- Development of a structured approach for the systematic generation of a number of design options at each level of process synthesis by employing P2 strategies, a number of thermodynamic tools, a process simulation tool and a quantitative environmental and cost evaluation tool.

- Development of a structured approach for the structural and parametric optimization of a flowsheet by the systematic use of a number of thermodynamic tools in combination with a process simulator and a quantitative environmental and cost evaluation tool.
- Development of a tool for quick quantitative evaluation of environmental and economic performance of a design option.
- Development of a new concept to carry out the life cycle environmental assessment of a design option separately in two domains: raw materials production and supply domain and gate-to-gate domain.
- Development of a ranking method for the normalization in the impact assessment phase of a life cycle assessment.

7.2 Recommendations for Future Work

In the present work, a number of methods and techniques have been developed to facilitate the implementation of the IP2M approach. However, further work is still required to develop a few tools and carry out some tasks, which would enable the designers to implement the IP2M approach completely and in efficient way. They are as follows:

- Development of a tool for the technical evaluation of a process flowsheet considering space requirement, flexibility of future modifications, simplicity in operation and maintenance.
- Development of an approach for the risk and safety evaluation of a process flowsheet.

- Development of an approach for multi-criteria optimization of a process flowsheet, which would enable handling of at least four objective functions.
- Integration of different tools used in IP2M such as SusDesign, E-Green, multi-criteria optimization, risk and safety evaluation and technical evaluation tools together in one common platform for the easy implementation of the IP2M.
- Integration of different databases with the IP2M tool to support its data requirement for the evaluation of different design options based on economic, environmental and technical criteria.
- Development of a probabilistic approach to reduce the data uncertainty associated with different evaluations.

Appendix A

Thermochemical Properties and Chemical Exergy of Selected Substances at 298 K and 1 atm

Substance	Enthalpy of Formation KJ/kmol	Gibbs Function of Formation, $\bar{g}$, KJ/kmol	Absolute Entropy $\bar{s}$ (KJ/kmol °K)
Carbon Monoxide	-110,530	-137,150	197.54
Carbon dioxide	-393520	-394380	213.69
Water (vapor)	-241820	-228590	188.72
Water	-285830	-237180	69.95
Oxygen	-249,170	231770	160.95
Nitrogen	472,680	455510	153.19
Methane	-74,850	-50,790	186.16
Propane	-103,850	-23,490	269.91
Butane	-126,150	-15,710	310.03
Ethane	-86680	-32890	229.49

Standard Molar Chemical Exergy

Substance	Model I	Model II
Nitrogen	640	720
Oxygen	3950	3970
Carbon dioxide	14,175	19,870
Water (vapor)	8,635	9,500
Water	45	900
Carbon monoxide	269,410	275,100
Methane	824,350	831,650
Ethane	1,482035	1,495,840

Appendix B-1

Calculation of Chemical Exergy of Methane at 25°C and 1 atmp Pressure

Complete combustion of hydrocarbon follows the following chemical reaction:

$$C_aH_b + \left(a+\frac{b}{4}\right)O_2 \rightarrow aCO_2 + \frac{b}{2}H_2O$$

For methane a = 1 and b = 4

As mentioned in Section, the chemical exergy of any hydrocarbon fuel is:

$$\bar{e}_F^{ch} = \left[\bar{g}_f + \left(a+\frac{b}{4}\right)\bar{g}_{o2} - a\,\bar{g}_{Co2} - \frac{b}{2}\bar{g}_{H2O(l)}\right](T_{o,}\,p_o) + a\,\bar{e}_{o2}^{ch} + \left(\frac{b}{2}\right)e_{H2O(l)}^{ch} - \left(a+\frac{b}{4}\right)\bar{e}_{o2}^{ch}$$

For methane, the above formula could be expressed as follows:

$$\bar{e}_{CH4}^{ch} = \left[\bar{g}_{CH_4} + 2\bar{g}_{o2} - \bar{g}_{Co2} - 2\bar{g}_{H2O(l)}\right](T_{o,}\,p_o) + \bar{e}_{o2}^{ch} + 2e_{H2O(l)}^{ch} - 2\bar{e}_{o2}^{ch}$$

Now putting the values of Gibbs function and chemical exergy of different components from appendix A. For chemical exergy values considering the values for model I, this gives the following values:

e_{CH4}^{ch} = -50,790 + 0 + 394,380 + 2 x 237,180 +14,135 + 2 x 45 -2 x 3,950

= 82,4315 KJ/kgmol

= 51391.20 KJ/kg

Appendix B-2

Typical Calculation of Chemical Exergy of a Flue Gas

Let us consider that at 1 bar pressure and 25°C temperature a flue gas contains 0.0510 mole fraction of water and 0.949 mole fraction of gaseous mixture. The composition of the gas mixture is as follows $yN_2 = 0.7910$, $yO_2 = 0.1446$, $yCO_2 = 0.0331$ and $yH_2O = 0.0313$ in mole fraction. Assume the flowrate and the overall molecular weight of the flue gas as 38.28 kg/sec and 28.25 respectively.

$$\mathbf{e_{ch}} = \sum \mathbf{yieich} + RTo \sum yiln(yi)$$

$$= 0.7910\,(640) + 0.1446(3950) + 0.0331(14175) + 0.0313(8635)$$

$$+ 8.314(298)[0.7910 \ln 0.7910 + 0.1446 \ln 0.1446 + 0.0331 \ln 0.0331$$

$$+ 0.0313 \ln 0.0313]$$

$$= 116.47 \text{ KJ/Kgmol}$$

Chemical Exergy of liquid water is 45KJ/kgmol (App-A)

Exergy of gas part is is: 116.47KJ/kgmol

So total exergy is: 116.47(.949) +45 (.0510) =112.82 kJ/Kgmol = 3.99 kJ/kg

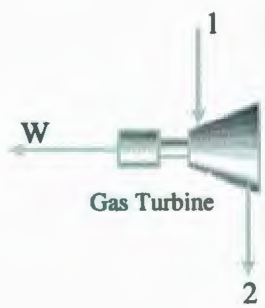
= 3.99 kJ/kg x 34.28 kg/sec = 152.27 kW

Appendix C

Typical Calculation of Exergy Destruction

Exergy Destruction in a Gas Turbine

Consider that the flue gas is entering the gas turbine as shown below at a flowrate of 38.05 kg/sec, and the workout put from the turbine is 30 MW.



The enthalpy and entropy values at 1 and 2 are obtained from Aspen-HYSYS, which are as follows:

h_1 = 218 kJ/kg , h_2 = -570.7 kJ/kg (in HYSYS enthalpy values are measured with respect to a reference value)

s_1 = 6.867 kJ/kg K and s_2 = 7.006 kJ/kg K

We know that exergy change between two states is (Section 2.8.2):

$$ef_1 - ef_2 = h_1 - h_2 - T_o(s_1 - s_2) + (V_1^2 - V_2^2)/2 + g\,(z_1 - z_2)$$

Neglecting the potential and kinetic energy effect and putting the values of the enthalpy and entropies.

Ef_1-Ef_2 = $\dot{m}$(218.3 +570.7) – 298 (6.867 -7.006)

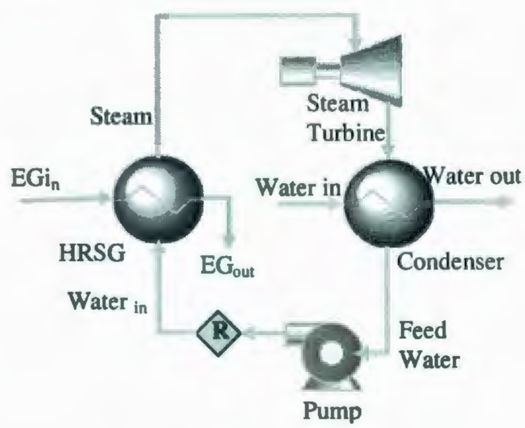
= 38.05 kg/sec X 830.422 kJ/kg = 31.597 MW

The exergy balance equation for the gas turbine is:

$\dot{m}(ef_1\text{-}ef_2) = \dot{W}_{cv} + \dot{E}_d$

Therefore, exergy destruction $\dot{E}_d$ = 31.597 – 30.0 = 1.567 MW, which is 4.96% of the input exergy to the gas turbine.

Exergy Destruction in a Heat Exchanger



The HRSG is shown in the above figure, EG_{in} and EG_{out} refer to exhaust gas in and out. The exergy given up by the exhaust gas is received by the $water_{in}$ which produces steam. Let us consider that the mass flowrate of the exhaust gas and water are 38.05 and 8.583 kg/sec respectively , therefore, exergy change between EG_{in} and EG_{out} is:

$\dot{m}\ (ef_1 - ef_2) = \dot{m}\ [h_1\text{-}h_2 - T_o\,(s_1\text{-}s_2)]$, where, points 1 and 2 refer to EG_{in} and EG_{out} streams.

$\dot{m}$ (ef_1 $-ef_2$) = 38.05 [(-570.7+1362) -298(7.006-5.816)] (data have been read from Aspen HYSYS)

$\dot{m}$ (ef_1 $-ef_2$) = 16.615 MW

Similarly, exergy change between steam and water$_{in}$ is:

$\dot{m}\ (ef_4 - ef_3) = \dot{m}\ [h_4 - h_3 - T_o(s_4 - s_3)]$

Where, points 3 and 4 refer to the water$_{in}$ and steam respectively.

$\dot{m}$ (ef_4 $-ef_3$) = 8.583[(-1.230E+4 + 1.58E+4)-298(9.393 -3.153)]

= 14.16 MW

The exergy balnce equation for the HRSG will be:

$\dot{m}\ (ef_1 - ef_2) = \dot{m}\ (ef_4 - ef_3) + \dot{E}_d$

Therefore, $\dot{E}_d$ = 16.615 – 14.16 = 2.449 MW

Thus, exergy destruction in the HRSG is (2.449/16.615)x100% = 14.74%

Appendix D

Calculation of Stoichiometric air-fuel ratio and λ for Methane Combustion

For complete combustion of methane following reaction is involved:

$$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$$

Therefore, 1 mole of methane reacts with 2 mole of Oxygen, which means that for the combustion of 16 kg of methane 64 kg O_2 is required. So, theoretically for the complete combustion of methane oxygen requirement is four times of methane.

We know that the amount oxygen present in dry air is 23.2% (by mass). Therefore, for the complete combustion of 1kg of methane required amount of air is:

4x 4.31 = 17.24

So, stoichiometric air fuel ratio for methane combustion is 17.24: 1

If at any condition, the actual air fuel ratio for the methane combustion is: 22:1, then the value of λ will be:

$$\lambda = \frac{\textit{Actual airfuel ratio}}{\textit{Stoichiometric airfuel ratio}} = \frac{22}{17.24} = 1.27$$

Appendix E-1

Cost Functions of Different Equipment

Following cost functions for different equipment were developed by equation fitting method.

Cost Function for Gas Turbine:

$Y = 18.928x^{1.2308}$

Where Y is the estimated cost in 2009 in dollar and x is the power in kW, this equation is good for the power range of 20 – 50 MW.

Cost Function for Compressor:

$Y = 25800x^{0.2238}$

Where Y is the estimated cost in 2009 in dollar and x is the power in kW, this equation is good for a small scale compressor having the power in the range of 20 – 150 kW. For large capacity compressor following cost equation has been used:

$Y = 211.97x^{1.0486}$

The above equation is valid within a range of 2500 -15000 kW

Cost function of Steam Turbine

$Y = 307.97x^{0.8409}$

Where, Y is the estimated cost of steam turbine with the associated condenser and x is the power in kW, this equation is valid within a power range of 750 – 14,000 kW.

Cost Function of Feed Pump

$$\mathbf{Y = 10.767\ x + 3289.7}$$

Where, Y is the estimated cost in 2009 and x is the pump power consumption in kW. The equation could be used for a range of 30 – 4500 kW.

Cost of the Heat Recovery Steam Generator (HRSG)

$$Y = 5413.7\ x^{0.3368}$$

Y is the estimated cost in dollar in 2009 and x is the heat transfer surface area in ft2 for a shell and tube type heat exchanger for large U value and CS-304 stainless steel material.

Cost Function of a Condenser for a Refrigeration Plant

$$Y = 2666.2\ x^{0.3961}$$

Where, Y is the estimated cost in dollar in 2009 and x is the heat transfer surface area in ft^2. The equation is good for air cooled bare tube area condenser in a range of 500 - 4500 ft^2, with medium U value and CS-304 stainless steel tube material.

Appendix E-2

Marshal and Swift Equipment Cost Index for Process Industries

Year	Annual Average
2008	1469.5
2007	1408
2006	1353.81
2005	1274.8
2004	1218.0
2003	1133.2
2002	1104.2
2001	1093.9
2000	1089.0
1999	1068.3
1998	1061.9

Appendix F

Technical Details of IRCH Index and Values for Selected Substances

The IRCH system assigns hazard scores between 0 and 200 based on the following algorithm:

Total Hazard Value = [(1.15 x **Worker Exposure Hazard Value**) + (**Environmental Hazard Value**/3.5)]/2

The components of the total hazard value include a wide variety of measures relating to a chemical's toxicity and physical-chemical properties such as vapor pressure, tendency to bioaccumulate, corrosivity, and so on.

Worker Exposure Hazard = (HVhealth x HVexposure) + (2 x HVsafety)

HVhealth = health effects hazard score, based on chronic and acute occupational toxicity measures

HVexposure = routes of exposure hazard value, based on chemical properties that indicate how exposure will occur (e.g. can the chemical be ingested, what is the ability of the chemical to form dusts or mists, etc.)

HVsafety = safety hazard value which considers a chemical's flammability, reactivity, and corrosivity

Environmental Hazard = HVwater+ HVair + HVland + HVglobal

HVwater = Hazrd value assigned according to UTN total hazard score (Davis et al., 1998)

HVair = sum of hazard values assigned if a chemical is a criteria pollutant, a hazardous air pollutant, a high risk pollutant, or an extremely hazardous substance

HVland= hazard value assigned according to its hazardous waste classification and characteristics

HVglobal = hazard value assigned if a chemical is a Class I or Class II ozone depleting substance

Table: IRCH index for selected Substance

Substance	IRCH Index
Butane	13
Carbon dioxide	4
Ethylene	19
Hydrogen sulfide	35
lead	33
Mercury	29
Nitric oxide	26
Nitrogen dioxide	27
Ozone	26
Propane	12
Sulfur dioxide	15
Zinc	11

Appendix G

Equations Used by E-Fast Software for Exposure Assessment

Estimation of Surface Water Concentrations

SWC (ppb) = [Release * CF_1 * (1 - WWT/100)] / [Stream flow * CF_2]

Where:

SWC = Surface water concentration (parts per billion or μg/liter);

Release = Chemical release to wastewater (i.e., pre-treatment release) (kilograms/site/day);

CF_1 = Conversion factor from kilograms to micrograms (10^9);

WWT = Removal in wastewater treatment (%);

WWT/100 = Converts wastewater treatment efficiency from a percentage to a fraction;

Stream flow = Measured or estimated flow of the receiving stream (million liters per day (MLD); and

CF_2 = Conversion factor from MLD to L/day (10^6).

Estimation of Drinking Water Exposures

To estimate how much of a given chemical a person will ingest through drinking water obtained from rivers and streams, E-FAST uses following Equations:

$$ADR_{POT} = \frac{SWC * (1 - DWT/100) * DWI * ED * CF1}{BW * AT}$$

$$ADD_{POT} \text{ and } LADD_{POT} = \frac{SWC * (1 - DWT/100) * DWI * ED * Reldays * CF1}{BW * AT * (365 \text{ days/yr})}$$

$$ADC \text{ and } LADC = \frac{SWC * (1 - DWT/100) * ED * Reldays * CF1}{AT * (365 \text{ days/yr})}$$

Where:

ADR_{POT} = Potential Acute Dose Rate (mg/kg/day);

ADD_{POT} = Potential Average Daily Dose (mg/kg/day);

$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day);

ADC = Average Daily Concentration in drinking water (μg/L);

LADC = Lifetime Average Daily Concentration in drinking water (mg/L);

SWC = Surface water concentration (ppb or mg/L);

DWT = Removal during drinking water treatment (%);

DWT/100 = Converts drinking water treatment efficiency from a percentage to a fraction;

DWI = Drinking water intake rate (L/day);

Reldays = Days of chemical release per year;

BW = Body weight (kg);

ED = Exposure duration (30 years for ADC, LADC, ADD_{POT}, and $LADD_{POT}$; one day for ADR_{POT});

AT = Averaging time (30 years for ADD_{POT} and ADC; 75 years for $LADD_{POT}$ and LADC; one day for ADR_{POT}); and

CF1 = Conversion factor of 0.001 mg/g.

The **harmonic mean** stream flow is used to calculate the ADD_{POT}, $LADD_{POT}$, ADC, and LADC. The **30Q5** stream flow is used to calculate the ADR_{POT}.

Estimating Exposures via Fish Ingestion

To estimate how much of a given chemical a person will ingest through eating fish, E-FAST uses the following formulas:

$$ADR_{POT} = \frac{SWC * BCF * ED * FI\ Intake * CF1 * CF2}{BW * AT}$$

$$ADD_{POT}\ \text{and}\ LADD_{POT} = \frac{SWC * BCF * FI\ Intake * ED * Reldays * CF1 * CF2}{BW * AT * (365\ days/yr)}$$

$$ADC\ \text{and}\ LADC = \frac{SWC * BCF * ED * Reldays * CF1 * CF2}{AT * (365\ days/yr)}$$

Where:

ADD_{POT} = Potential Average Daily Dose (mg/kg/day);

ADR_{POT} = Potential Acute Dose Rate (mg/kg/day);

$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day);

ADC = Average Daily Concentration in fish tissue (mg/kg); and

LADC = Lifetime Average Daily Concentration in fish tissue (mg/kg).

SWC = Surface water concentration (ppb or μg/L);

BCF = Estimate of chemical's bioconcentration potential (L/kg);

FI intake = Fish Ingestion Rate (g/day);

Reldays = Days of chemical release per year;

BW = Body weight (kg);

ED = Exposure duration (30 years for ADC, LADC, ADD_{POT}, and $LADD_{POT}$;

one day for ADR_{POT});

AT = Averaging time (30 years for ADC and ADD_{POT}; 75 years for LADC and $LADD_{POT}$; one day for ADR_{POT});

CF1 = Conversion factor of 0.001 mg/g; and

CF2 = Conversion factor of 0.001 kg/g.

Estimation of Drinking Water Exposures

To estimate how much of a given chemical a person will ingest through drinking groundwater, E-FAST uses the following formula:

$$ADD_{POT} / LADD_{POT} = \frac{GWC * (1 - DWT/100) * DWI * EF * ED}{BW * AT * (365\ days/yr)}$$

$$ADC / LADC = \frac{GWC * (1 - DWT/100) * EF * ED}{AT * (365\ days/yr)}$$

Where:

ADD_{POT} = Potential Average Daily Dose (mg/kg/day);

$LADD_{POT}$ = Potential Lifetime Average Daily Dose (mg/kg/day);

GWC = Ground water concentration (mg/L);

ADC = Average Daily Concentration in drinking water (mg/L);

LADC = Lifetime Average Daily Concentration in drinking water (mg/L);

DWT = Removal during drinking water treatment (%);

DWT/100 = Converts drinking water treatment efficiency from a percentage to a fraction;

DWI = Drinking water intake rate (L/day) (U.S. EPA, 1997);

EF = Exposure frequency (assumes 365 days/yr for all calculations);

BW = Body weight (adult) (kg) (U.S. EPA, 1997);

ED = Exposure duration (30 years for ADD_{POT} and $LADD_{POT}$); and

AT = Averaging time (30 years for ADC and ADDPOT; 75 years for LADC and $LADD_{POT}$).

Estimation of Air Concentrations from Stack Releases

E-FAST uses a simple, conservative method for estimating ambient air concentrations that may result from air emissions from sources with tall stacks such as boilers and incinerators. Maximum annual average ground level air concentrations are predicted using a derived relationship between release amount and maximum annual average concentration that was developed by OPPT using Industrial Source Complex - Long Term (ISCLT) modeling of emissions from a hypothetical facility. This hypothetical facility has a stack height of 30 meters, a stack diameter of 1.5 meters, an exit gas temperature of 400 K, and an exit velocity of 5 m/sec. The hypothetical facility was modeled using actual meteorological data for a city expected to produce relatively high concentrations, mostly because of the persistent wind directions in the area. The human receptor is assumed to be located 1,000 meters downwind from the stack because the ISCLT modeling showed that maximum concentrations occurred at this distance and because 1,000 meters is a reasonable distance from a facility with a tall stack at which one might expect residences to be located.

$C = (Q_{yr}) * (3 \times 10^{-9})$

Where:

C = Predicted maximum annual average concentration in air (mg/m^3); and

Q_{yr} = Chemical release rate (kg/site-yr).

Estimation of Inhalation Exposures to Stack and Fugitive/Vent Releases

E-FAST uses the following equations to calculate exposures associated with stack releases.

$$LADD_{POT} \text{ and } ADD_{POT} = \frac{Q_{yr} * F * Factor * IR * ED}{BW * AT * (365 days/yr)}$$

$$LADC \text{ and } ADC = \frac{Q_{yr} * Factor * ED}{AT}$$

Where:

Q_{yr} = Chemical release rate (kg/site-yr);

F = Number of release days per year (days/yr) (assumed to be 365 days/yr);

Factor = 3E-09 (mg-yr)/(m^3-kg)

IR = Inhalation rate (m^3/day);

ED = Exposure duration (30 years for ADC, LADC, ADDpot and LADDpot);

BW = Body weight (kg); and

AT = Averaging time (30 years for ADDpot and ADC; 75 years for LADDpot and LADC)

Appendix H

Risk Characterization

Carcinogenic Risk

Carcinogenic risk is defined as the chronic daily intake dose developed by the exposure assessment multiplied by the carcinogenic slope factor.

Risk = I_c x SF

Where, I_c = chronic daily intake of carcinogen (mg/kg.day)

SF = carcinogen slope factor (kg.day)/mg

Noncarcinogenic Risk

Noncarcinogenic risk is characterized in terms of hazard index. This is defined as the ratio of the estimated intake dose from the exposure assessment to the reference concentration.

HI = I_N / Rfc

Where, HI = hazard index

I_N = chronic daily intake of non-carcinogen (mg/kg.day)

Rfc = reference concentration

Hazard index less than 1 is acceptable. In case of exposure of multiple chemicals the hazard index must be calculated for each chemical of concern for all pathways and exposure routes. For the exposure of multiple non-carcinogens chemicals the corresponding hazard index of each chemical is usually summed up to provide the final risk score for all the chemicals.