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Systematic Framework for Multiobjective Optimization in Chemical Process Plant Design

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1. Introduction

For solving multiobjective decision making problems, a systematic and effective procedure is required. As far as the process or control system has to be modified process simulators like Aspen Plus™, Aspen Dynamics are widely used. But these simulators are not designed for investigation of other objectives as environment and safety. Due to complex and conflicting nature of multiobjective decision making an integrated optimization tool should be of value. In this chapter a systematic methodology based on independent modules and its different stages to deal this problem is presented in detail.

2. Proposed methodology

The methodology is built around several standard independent techniques. These techniques have been suitably modified/adopted and woven together in an integrated platform. The main aim is to standardize the screening and selection of decisions during design/modification of chemical process plant and optimizing the process variables in order to generate a process with improved economics along with satisfaction of environmental and safety constraints. The methodology (see Figure 1) consists of four layers/stages:

- Generation of alternatives and problem definition;
- Analysis of alternatives i.e. generation of relevant data for comparison of Environmental, economic and safety objectives
- Multiobjective decision analysis/ optimization
- Design evaluation stage i.e. decision making from the pareto-surface of non-inferior solution or ranking of alternatives

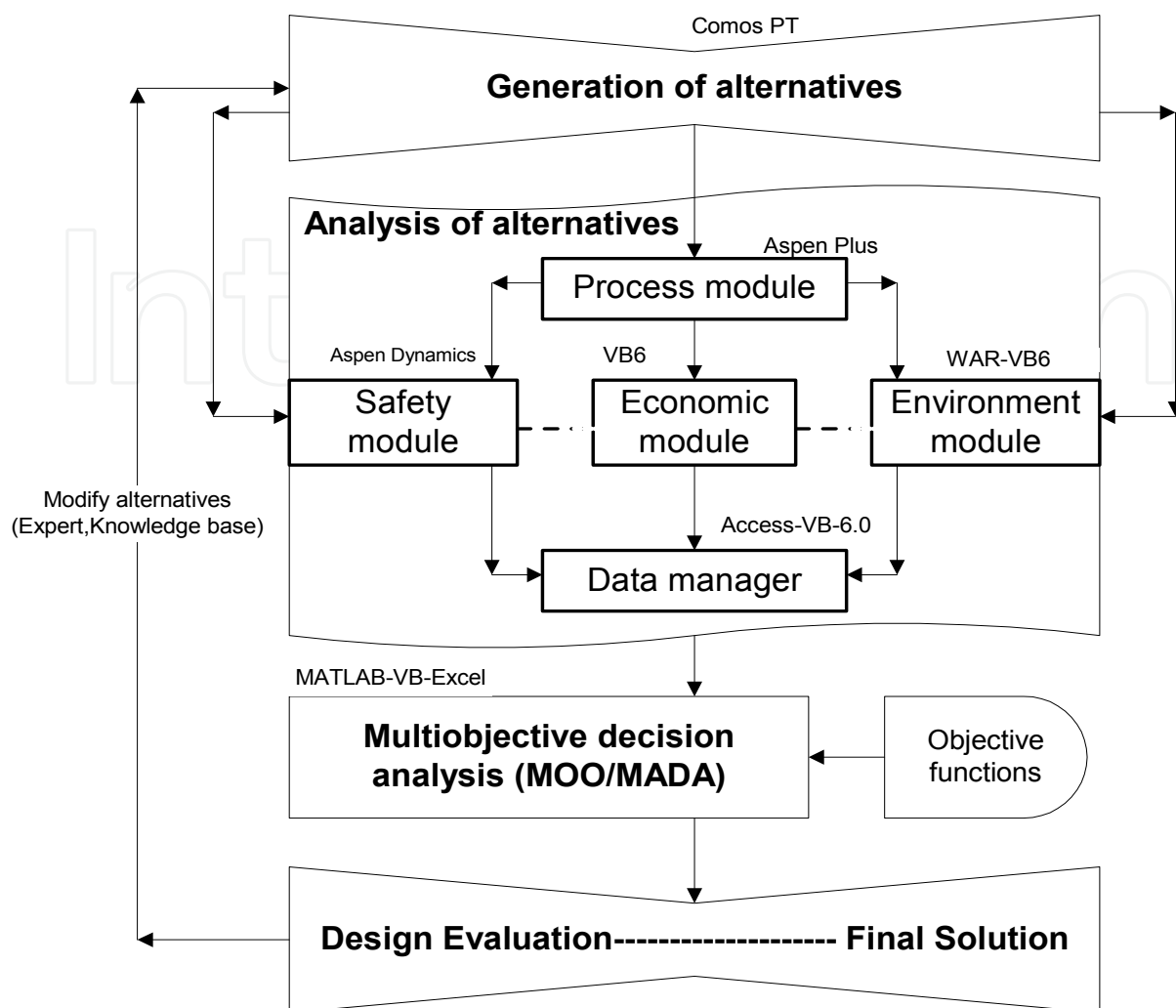


Fig. 1. Simplified block diagram of proposed methodology

2.1 Stage I: Generation of alternatives and problem definition

The first layer composed of following tasks:

- Definition of the scope of the study,
- Statement of key assumptions and the performance targets such as quality etc.,
- Degree of freedom analysis,
- Identification of the key design, control, and manipulated variables,
- Definition of the system boundary,
- Identification of constraints,
- Choice of functional unit for all calculations,
- Collection of relevant information about process and chemicals to be handled,
- Generation of different alternatives either based on suggestion from independent departments or using the individual objective modules from stage II.

Seader et al. (1999)[6] has described rules for selection of process variables in the book "Process design principles-synthesis, analysis and evaluation". The data and information

about the process and chemicals involved such as thermodynamic and kinetic data can be found from journal articles, patents or handbooks. Current chemical prices can be obtained from market reports if not available in main plant documentation or company central data base. In addition to these sources, some data related to quantification of environmental impacts and material safety data sheets of chemical are also collected from commercial data bases so that an impact assessment and safety analysis can be performed in subsequent design steps. Commercial computer aided tool like Comos^{PT} can be used for plant documentation and to support stage-I of proposed methodology.

2.2 Stage II: Analysis of alternatives

This stage is composed of independent modules used to generate relevant information for evaluation of economic, safety and environmental performance objectives. These modules are:

- Process module
- Safety module [1,3]
- Economic module
- Environment module [2]
- and a data manager for managing the relevant information generated from these modules.

2.3 Process module

In the process module, an operation model of the process system has to be developed for evaluating alternatives. The configured simulation model has to be able to reproduce the selected results to an accepted degree of accuracy. This simulation model can be used for design and operation, revamping and debottlenecking of the process under study[7]. Three major integrated simulation systems widely used in the firms and companies for this purpose are Aspen technology (Aspen Plus, Aspen dynamics etc), Hyprotech (Hysys process, Hysys plant etc) and Simulation Sciences (Pro/II etc.). Aspen PlusTM 12.1 is used in this work for development of simulation model and linked in a visual basic platform for integration with safety, economic and environment modules. The most important results available from the process simulation model are material and energy balance information for both streams and units, rating performance of units and tables and graphs of physical properties. A brief description of Aspen PlusTM 12.1 and steps involved in development of the process simulation model is described here below.

Aspen PlusTM

Aspen PlusTM supports both sequential modular and equation oriented computation strategy and allows the user to build and run a steady-state simulation model for a chemical process. It provides a flexible and productive engineering environment designed to maximize the results of engineering efforts, such as user interface mode manager, quick property analysis, rigorous and robust flowsheet modelling, interactive architecture, powerful model analysis tools and analysis and communication of results. Therefore, it lets the user to focus his/her energies on solving the engineering problems, not on how to use the software. It is not only good for process simulation but also allows to perform a wide

range of other tasks such as estimating and regressing physical properties, generating custom graphical and tabular output results, sensitivity analysis, data-fitting plant data to simulation models, costing the plant, optimizing the process, and interfacing results to spreadsheets.

The development of a simulation model for a chemical process using Aspen Plus™ 12.1 involves the following steps (see details in table 1):

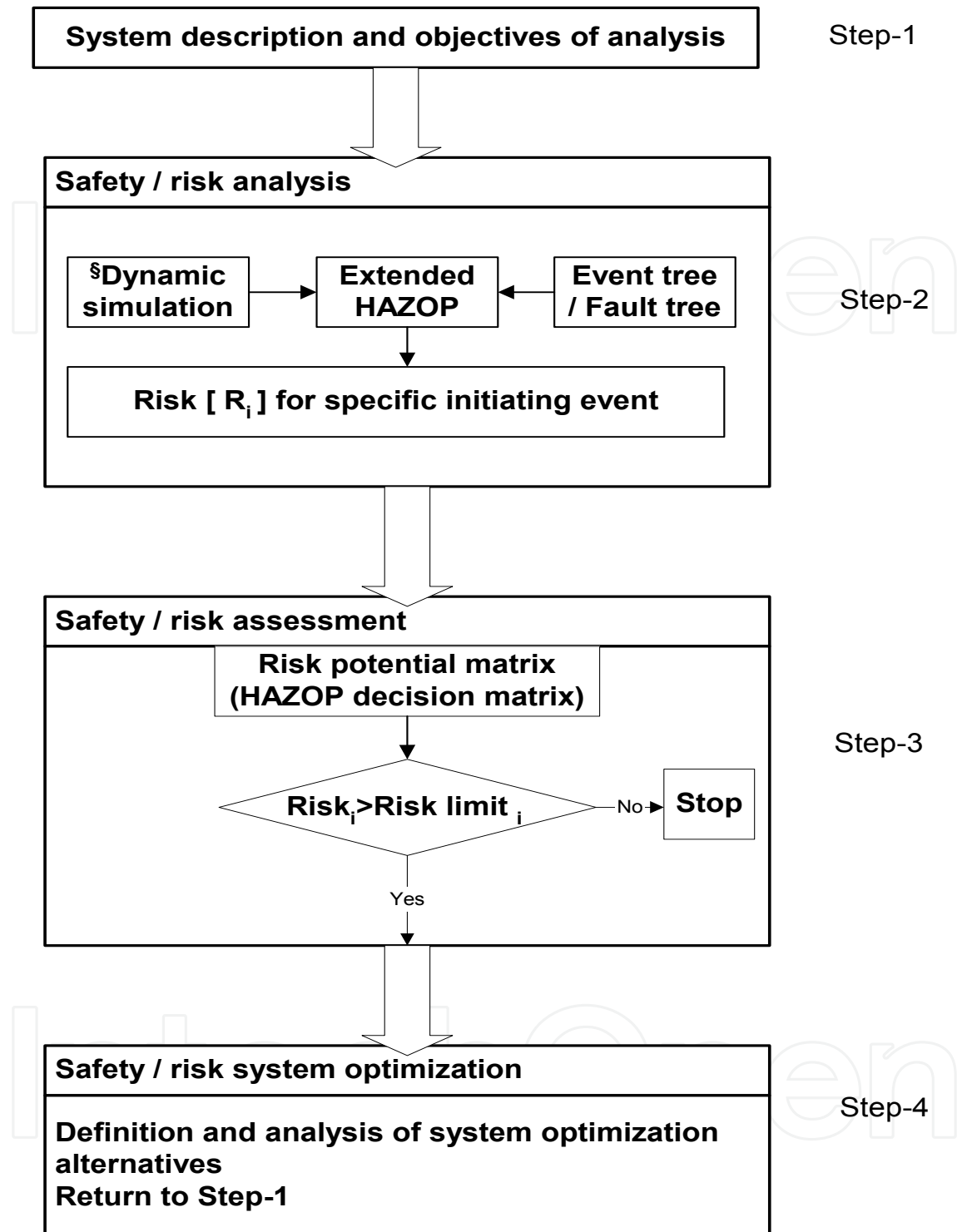
1. Define the process flowsheet configuration by specifying
 - Unit operations
 - Process streams flowing between the units
 - Unit operation models to describe each unit operation
2. Specify the chemical components,
3. Choose a thermodynamic model to represent the physical properties of the components and mixtures in the process,
4. Specify the component flow rates and thermodynamic conditions (i.e. temperature, pressure, or phase condition) of the feed streams,
5. Specify the operating conditions for the unit operations,

Step	Used to
Defining the flowsheet	Break down the desired process into its parts: feed streams, unit operations, and product streams
Specifying stream properties and units	Calculate the temperature, pressure, vapor fraction, molecular weight, enthalpy, entropy and density for the simulation streams
Entering components	From a databank that is full of common components
Estimating property parameters	Property Constant Estimate System (PCES) can estimate many of the property parameters required by physical property models
Specifying streams	Streams connect unit operation blocks in a flowsheet and carry material and energy flows from one block to another. For all process feed streams, we must specify flowrate, composition, and thermodynamic condition
Unit operation blocks	We choose unit operation models for flowsheet blocks when we define our simulation flowsheet

Table 1. Developmental process for an Aspen Plus™ simulation model

2.4 Safety module

Safety module is based on combination of conventional standard risk analysis techniques and process disturbance simulation. This module not only generates relevant information related to safety aspects for multiobjective decision analysis but also used for safety/risk analysis and optimization. The purpose of this module is to determine risk from operational disturbances and to develop effective risk reductions. It can be divided into the following steps (Figure 2):



§ Simulation of process related malfunctions

$i = \{ \text{financial risk , environmental risk , human health risk} \}$

Step 1: System description and objectives of analysis (before starting safety and risk analysis)

Step 2: Safety/risk analysis (identification of weak points via Extended HAZOP)

Step 3: Safety/risk assessment (categorization of risk via risk potential matrix (HAZOP decision matrix))

Step 4: Safety/risk system optimization

Fig. 2. Simplified block diagram of safety module

2.4.1 Step 1: (Before starting safety/risk analysis) - Description of system and objectives of analysis

For efficient safety/risk studies, the analyst must have an accurate description of the system to be investigated and a clear objective of the analysis study. Therefore, in this step the purpose, objectives, and scope of the study are clearly defined. The necessary information required for the study such as process flow diagrams, piping and instrumentation diagrams, plant layout schematics, material safety data sheets, equipment data sheets, operating instructions, start up and emergency shutdown procedures, and process limits, etc. is gathered from plant documentation. A team under a trained and experience leader with five to seven people including experts of the design and operation of the subject process may be formulated.

2.4.2 Step 2: Safety/risk analysis (Identification of weak points via extended HAZOP) - Extended HAZOP

Our intention is to identify weak points due to disturbances in operation, which may or may not be hazardous, in order to improve safety, operability, and/or profit at the same time. Extended HAZOP (HAZOP supported by dynamic simulation, event tree and fault tree techniques and HAZOP decision matrix) is used not only for identification of weak points but also for generation and analysis of optimization proposals [8-11]. Extended HAZOP differs from the standard HAZOP approach in following aspects:

i. Use of dynamic simulation:

In Extended HAZOP, the analysis of the influence of disturbances (failures) on the behaviour of the process is based on shortcut or simplified hand calculations or dynamic simulation. Aspen dynamics is used for this purpose.

ii. Classification of risk related consequences:

Each established consequence (hazard) has to be expressed by a consequence class (C). The plant specific scoring (from 0 (lowest) to 8 (highest)) chart is given in Table 2 (a & b) based on principle consequence analysis. For classification of consequences based on principle release estimates, accident consequence analysis techniques (models for calculation of toxic, fire and explosion effects) and plant location data (capital investment, population density etc.) have to be considered.

Illustrative Example 1

Figure 3 shows the plant lay out considered for developing plant specific consequence scoring chart. The area around the plant is open fields (rural condition). As weather conditions changed around the year, so certain assumptions are made to results in worse case conditions for consequence analysis. These include weather conditions and wind speed that result in smallest value of dispersion coefficients. Therefore, stability "F" and wind speed as low as possible (1.5 m/s) is selected. It is assumed that 10 workers are present (working 24 h each day), which are not distributed uniformly, on the land in area (100 m x 100 m) around the column under study. Acetone is selected as representative fluid for consequence analysis.

Acetone vapours released from the vent line at a rate of 1616 kg/h due to loss of cooling medium. It is assumed that released vapours form a cloud for 30 minutes before being

Effects	Class	Financial loss (€)	Class related consequences: examples
Function impairment	*	< 10	: Product quality lowering (brief)
	1	10 ¹ - 10 ²	: Product quality lowering
	2	10 ² - 10 ³	: Product quality lowering (long term)
Functional Loss	3	10 ³ - 10 ⁴	: Production disturbance (brief) Soil contamination Safe dispersion of material release from vent line
	4	10 ⁴ - 10 ⁵	: Production disturbance Material release from the piping Pump damage (pressure impacts)
	5	10 ⁵ - 10 ⁶	: Production disturbance (long term) Jet fire as result of release of material from vent line Pool fire (from pump leakage)
Safety and Environmental pollution	6	10 ⁶ - 10 ⁷	Fireballs due to catastrophic rupture of vapour product line
	7	10 ⁷ - 10 ⁸	Vapour cloud explosion (ignoring domino effect)
	8	>10 ⁸	Vapour cloud explosion along with domino effect
Effects	Class	Community	Class related consequences: examples
Function impairment	*	No effect on people	: Product quality lowering (brief)
	1	Nuisance effect	: Product quality lowering
	2	Minor irritation effect to people & local news	: Product quality lowering (long term)
Functional Loss	3	Moderate irritation effect to people and non compliance to laws, local news	: Production disturbance (brief) Soil contamination Safe dispersion of material release from vent line
	4	Moderate irritation effects to people & environment, single injuries and regional news	: Production disturbance Material release from the piping Pump damage (pressure impacts)
	5	Significant effects to people and environment, > 1 injuries & regional news	: Production disturbance (long term) Jet fire as result of release of material from vent line Pool fire (from pump leakage)
Safety and Environmental pollution	6	Major effects to people and environment, multiple injuries, fatality likely, regional news	Fireballs due to catastrophic rupture of pipe or condenser (vapour product line)
	7	Severe effects to people and environment, fatality, regional news	Vapour cloud explosion (ignoring domino effect)
	8	Multiple fatalities and process shutdown certain, international news	Vapour cloud explosion along with domino effect

Environment and Health consequences

Table 2. Scoring chart for Consequence Financial consequences [3.4]

← 5 km

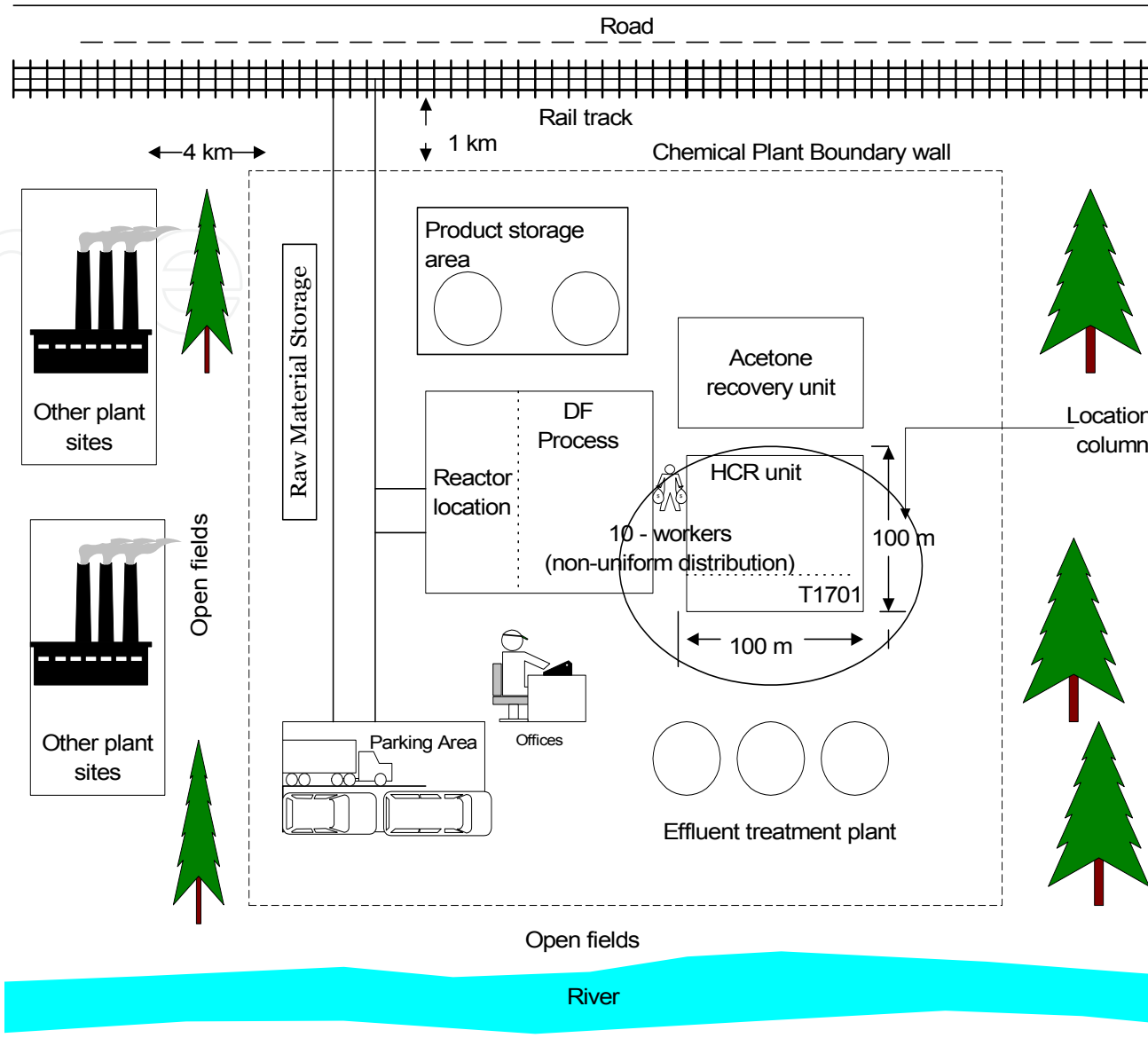


Fig. 3. Plant lay out for establishing consequence score chart

ignited and leads to vapour cloud explosion. The physical effects of this scenario or event is calculated as:

Weight of fuel in the cloud= $M = 1616 / 2 = 808$ kg

Then amount of TNT equivalent to the amount of this flammable material is

$$M_{TNT} = \alpha \cdot \frac{M \cdot H_c}{H_{TNT}}$$

Where α = explosion efficiency ~ 0.05 (Cameron 2005) H_c = heat of combustion of fuel $\sim 3.03 \times 10^4$ kJ/kg for acetone

H_{TNT} = TNT blast energy ~ 5420 kJ/kg; so $M_{TNT} = 225.25$ kg

Then, using relation $Z = R / (M_{TNT})^{1/3}$ and figure 4, scaled distance and overpressure is estimated. Table 3 presents the results obtained.

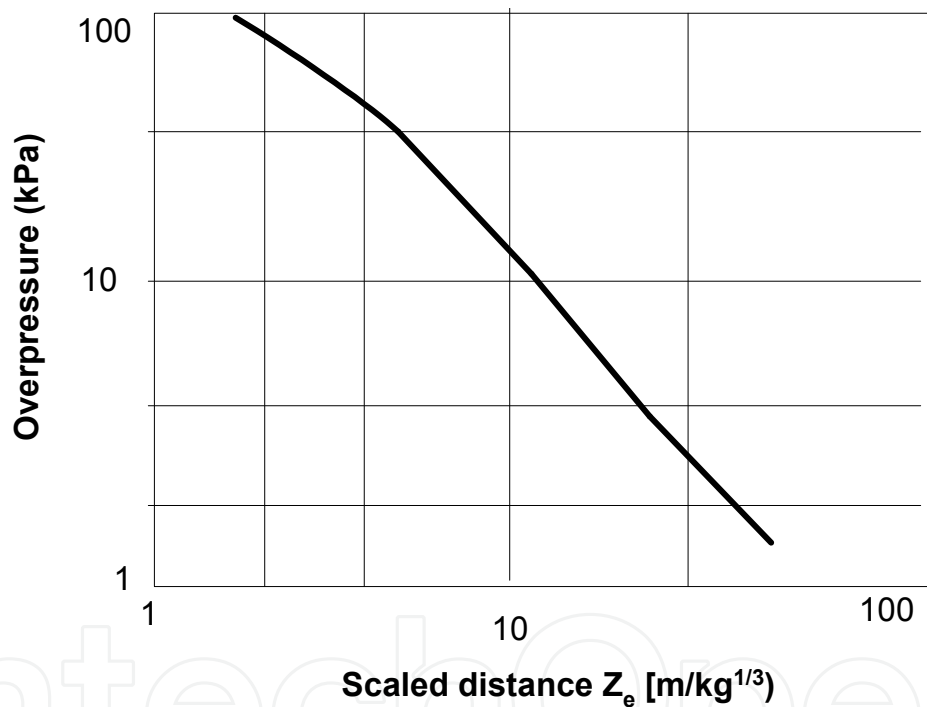


Fig. 4. Overpressure versus scaled distance for TNT explosions on flat surfaces (Tweeddale 2003, p. 115)

Distance, R M	Scaled distance, Z m / kg ^{1/3}	Overpressure, Δp kPa
10	1.64	90
20	3.28	40
50	8.21	20
100	16.40	7

Table 3. Results of physical effects of vapour cloud explosion

It is estimated that severe structural damage and 15 % chance of fatality outdoors or 50 % chance indoor will be experienced out to 20 m and almost complete destruction of all ordinary structures and 100 % chance of fatality indoors to 10 m distance.[8] (see Cameron 2005, p. 268).

iii. Classification of frequencies of risk related consequences:

The frequency of occurring for each possible consequence (hazard) has to be expressed by a frequency class, called (F) according to the scoring chart for frequency (Table 3.4). Definition of frequency class may be supported by Event Tree and/or Fault tree analysis techniques or Layer of protection analysis (LOPA) or historical databases.

For establishing frequency class: Estimation / calculation of frequency of vapour cloud explosion and fatality of person because of release of material due to catastrophic rupture of distillation column.

Frequency of catastrophic rupture of column = 10^{-6} (Taken from table 4)

Class	Frequency of occurring incident		
	Frequency 1/y	Comprehension	Examples based on general data bases
9	$<10^{-8}$	Very very small	Catastrophic rupture or leakage of pipe of diameter > 150 mm
8	$10^{-8} - 10^{-7}$	Very small	Catastrophic rupture of pipe of diameter ≤ 50 mm
7	$10^{-7} - 10^{-6}$	Small	Catastrophic rupture of fractionating system (excluding piping), storage tank rupture
6	$10^{-6} - 10^{-5}$	Less small	Pipe residual failure, 100 m full breach, Double wall tank leakage
5	$10^{-5} - 10^{-4}$	Moderate	Process vessel leakage of ≥ 1 mm diameter
4	$10^{-4} - 10^{-3}$	Less moderate	Pump leakage , Heat exchanger leakage
3	$10^{-3} - 10^{-2}$	Less high	Safety valve open spuriously, Large external fire
2	$10^{-2} - 10^{-1}$	High	Cooling water failure, BPCS instrument loop failure
1	$10^{-1} - 10^0$	Very high	Operator failure, Regulator failure , Solenoid valve failure
*	$>10^0$	Very very high	Power failure in developing countries, Operators failure under high stress

Table 4. Scoring chart for frequency [3.4]

Probability of ignition of released material = 0.10 (CCPs 2000, Borysiewich 2004)

Probability of VCE if released material ignited = 0.01 (CCPs 2000, Borysiewich 2004)

Probability of fatality of a person exposed to overpressure of 40 kPa due to VCE = 0.20 (Tweeddale 2003, p. 117 Figure 5-14)

Then, frequency of vapour cloud explosion = $10^{-6} \cdot 0.10 \cdot 0.01 = 10^{-9}$

So frequency class for this scenario = 9

Frequency of fatality of a person exposed to VCE = $10^{-9} \cdot 0.20 = 2 \cdot 10^{-10}$

So frequency class for this scenario = 9

iv. Way of documenting the HAZOP results

The Extended HAZOP methodology worksheet for documenting the HAZOP team results is shown in Figure 5. Below consequence the physical effects and risk has to be documented first and next risk has to be classified using score charts (Table 3.2) related to financial, environment and health related consequences. The worst score of each risk has to be documented. For each risk related consequence, frequency class has also to be established.

Consequence, €		<10	10 ¹ - 10 ²	10 ² - 10 ³	10 ³ - 10 ⁴	10 ⁴ - 10 ⁵	10 ⁵ - 10 ⁶	10 ⁶ - 10 ⁷	10 ⁷ - 10 ⁸	>10 ⁸
		* F	1	2	3	4	5	6	7	8
>10 ⁰	*									
10 ⁻¹ - 10 ⁰	1									
10 ⁻² - 10 ⁻¹	2									
10 ⁻³ - 10 ⁻²	3									
10 ⁻⁴ - 10 ⁻³	4									
10 ⁻⁵ - 10 ⁻⁴	5									
10 ⁻⁶ - 10 ⁻⁵	6									
10 ⁻⁷ - 10 ⁻⁶	7									
10 ⁻⁸ - 10 ⁻⁷	8									
<10 ⁻⁸	9									
		Immediate action needed before further operation								
		Action at next occasion after qualification of analysis for improving system								
		Optional								
		No further action needed								

Fig. 5. Risk potential matrix (Extended HAZOP decision matrix)

Illustrative Example 2

Release of material to atmosphere from vent line or vapour line may disperse safely or has toxic effects or can lead to several outcomes such as flash fire, vapour cloud explosion and fire balls. So documenting consequence class in HAZOP work sheet, the score '8' of the most severe consequence will be documented.

Plant/P&ID :		Process:				Document:		
Equipment :		Function:				Page :		
Volume :						Date :		
No	Guide word / Process Parameter	Detection/ Safeguards	Possible causes	Consequences	FC	Recommended Actions	FC	Resp./ Ref.
				Physical effects: Risk related:				

1- Short cut calculations 2-Dynamic simulation 3-deterministic models 4- Event tree 5- Fault tree
6- Historic data base

2.4.3 Step 3: Safety/risk assessment - Risk potential matrix (HAZOP decision matrix)

Figure 6 shows the risk potential matrix (HAZOP decision matrix) used for order of magnitude ranking of events. The rows of the matrix consider frequency class, while the columns show the consequence class. Each cell in the matrix represents a risk category. For the decision process, the matrix is divided into four risk category levels.

Risk level I --- red area --- scenario in this level is intolerable and immediate action (plant or process modification) is needed to reduce that risk category or more detailed quantified analysis has to be carried out in order to find arguments for wrong preliminary decisions.

Risk level II --- grey area --- scenario in this level is tolerable but not acceptable for long period of time so action at next schedule maintenance is needed to reduce that risk category.

Risk level III --- yellow area --- scenario in this level is acceptable and any action to reduce that risk category is optional.

Risk level IV--- green area --- scenario in this level needs no action.

Risk potential matrix (HAZOP decision matrix) may be also used for:

- Documentation of the status of the plant safety
- Selection and development of optimization proposals
- Importance of improvement
- Documentation of improvement achieved

The application of risk potential matrix (HAZOP decision matrix) in the Extended HAZOP is shown in figure 5. Arrows show the transformation of entries from the Extended HAZOP worksheet to the HAZOP decision matrix. The identity number (ID) of each scenario of the Extended HAZOP worksheet is placed in HAZOP decision matrix. Recommended actions for this scenario will be placed from Extended HAZOP sheet to the bottom of HAZOP decision matrix. First HAZOP decision matrix will shows the existing status and second HAZOP decision matrix shows the improved plant status after recommended actions.

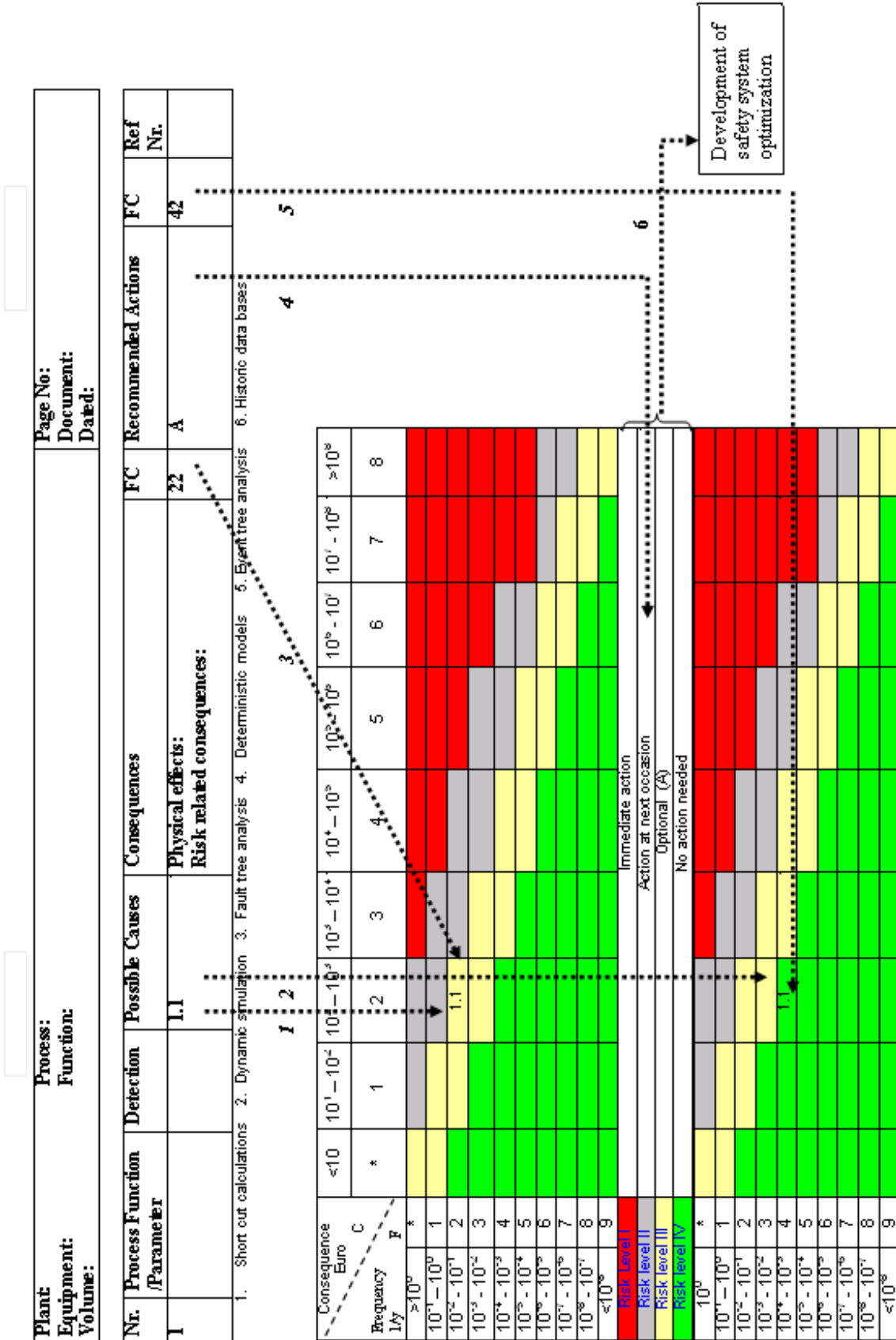


Fig. 6. Application of HAZOP decision matrix in Extended HAZOP

Similarly all results from Extended HAZOP worksheets are transferred to the HAZOP decision matrix. Keeping in view the risk target and depending on the scenario or recommended actions during the Extended HAZOP discussion, analysis team may reach a safety related modification proposal. Next, if safety/ risk optimization is in focus then weak points/scenarios with similar risk are clustered after analyzing HAZOP decision matrix and safety related optimization proposals are developed.

2.4.4 Step 4: Safety/risk system optimization (Development and analysis of optimization proposals)

In this step, safety related optimization proposals are generated and evaluated using dynamic simulation, Event tree analysis and/or Fault tree analysis. The optimization proposals can be developed at two levels:

- Simple optimization proposals e.g. addition of pressure alarm or change of location of sensor within the Extended HAZOP discussion
- Optimization proposals related to severe scenarios by evaluating risk potential matrix (HAZOP decision matrix)

The relevant information such as frequency and damage data will be transferred to economic module for safety related cost calculations and multiobjective decision making (if more than one alternatives developed).

2.5 Economic module

In all stages of design process, economic evaluation is crucial for the evaluation of process alternatives. Various objective functions are available in the literature of chemical engineering economics for economic evaluation of chemical processes. Some quite elegant objective functions, which incorporate the concept of the „time value of money“, are net present value (NPV) and discounted cash flow. Business managers, accountants and economists prefer these methods because they are more accurate measures of profitability over an extended time period. However, application of these methods needs certain assumptions[12]. Total annualized cost (TAC) can be used as economic indicators/objective function for the evaluation of design alternatives and economic optimization.

Economic module developed in Visual Basic consists of two distinct sections. First section carries out standard cost calculations (i.e. Fixed capital investment (FCI) and operational cost (OC1)) and compute total annualized cost (TAC1) while second section carries out extended cost calculations i.e. process safety/risk related costs and computes the fixed capital investment related to safety system (FCISS), accident and incident damage related risk cost. Table 3.5 illustrates the difference of cost elements considered in standard practice of cost calculations of chemical process design and in this economic module. Figure 7 shows the simplified block diagram of economic module.

2.5.1 Standard cost calculations

Standard cost calculations involves fixed capital investment (FCI1) and operational cost (OC1). Fixed capital investment (FCI1) includes the cost of design and other engineering and construction supervision, all items of equipment and their installation, all piping,

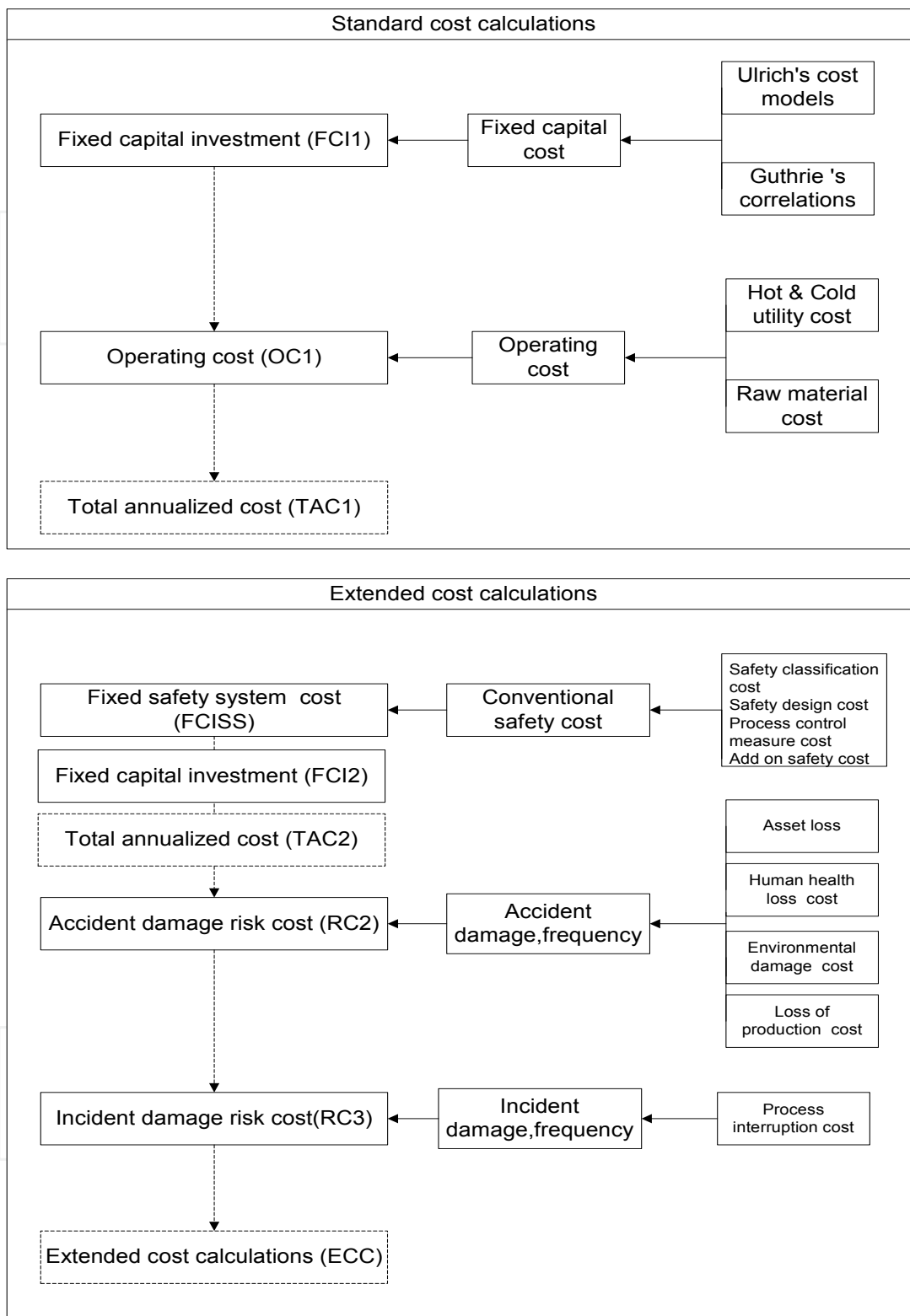
Standard cost calculations	Economic module used in this work
<ul style="list-style-type: none"> • FCI1 = Fixed capital investment using either cost equations that have been derived by Ulrich or correlations developed by Guthrie depending on users choice • OC1= Operating cost (including both direct (e.g. raw material, utilities etc.) and indirect costs (e.g. taxes, overhead cost etc) • TAC1 = total annualized cost = $d \cdot (FCI1) + OC1$ normally d is taken 0.15-25 but can also be computed using depreciation calculation methods 	<ul style="list-style-type: none"> • FCI1= Fixed capital investment using either cost equations that have been derived by Ulrich or correlations developed by Guthrie depending on users choice • FCI2= FCI1 + fixed capital investment related to safety system (FCISS) • OC1= Operating cost (including both direct (e.g. raw material, utilities etc.) and indirect costs (e.g. taxes, overhead cost etc) • TAC1 = total annualized cost = $d \cdot (FCI1) + OC1$ • TAC2 = total annualized cost = $d \cdot (FCI2) + OC1$ normally d is taken 0.15-25 but can also be computed using depreciation calculation methods <p>Extended cost calculations</p> <ul style="list-style-type: none"> • RC1 = risk cost 1= Asset risk cost + health risk cost + environmental risk cost • RC2 = risk cost2 = RC1+ production loss risk cost • RC3 = risk cost3 = process interruption cost • TRC = total risk cost = RC2+RC3 • ECC = Extended costs

Table 5. Elements of economic module and difference from standard cost calculations

instrumentation and control systems, buildings and structures, and auxiliary facilities such as utilities, land and civil engineering work. Several capital cost estimate methods ranging from order of magnitude estimate (ratio estimate) to detailed estimate (contractors estimate) are used for the estimation of installed cost of the process units in the chemical plant.

The most commonly used method that provides estimates within 20-30% of actual cost and widely used at design stage involve the usage of cost charts/correlations (Guthrie's article (1969) and book (1974), chapter 5 of Ulrich's 'A guide to chemical engineering process design and economics' (1984), 'Plant design and economics for chemical engineers' by Peters and Timmerhouse (1991)) for estimating the purchase cost of major type of process equipment [13-15].

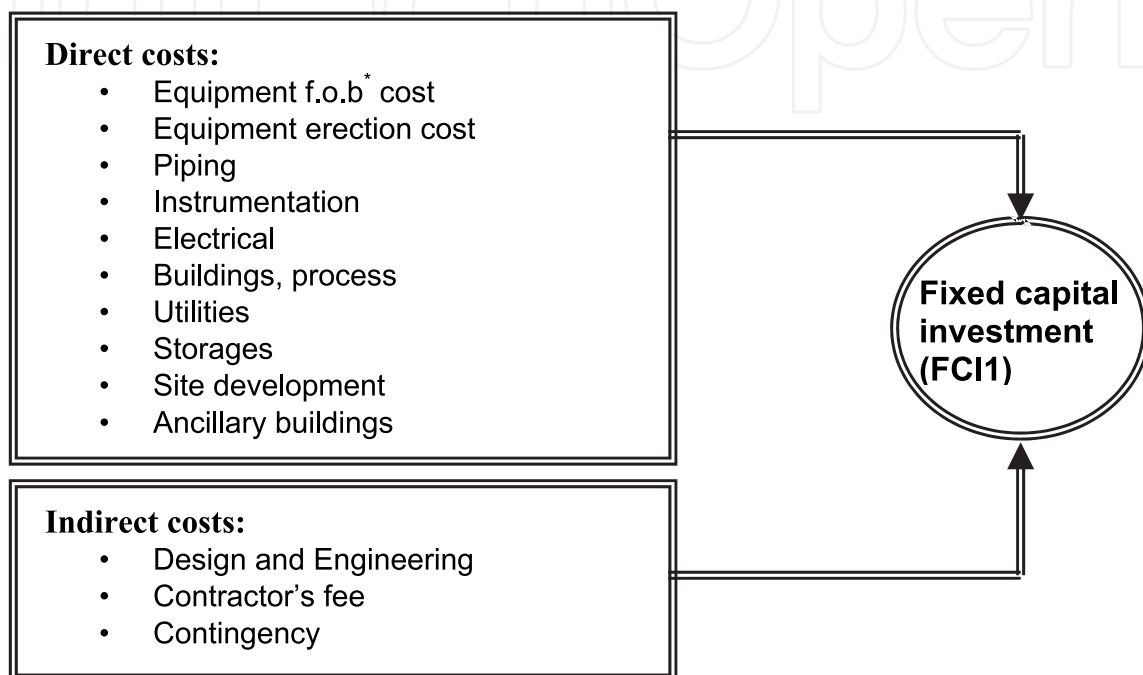
These cost charts / correlations were assembled in the 1960's or earlier and are projected to the date of installation using cost indices or escalation factors such as the chemical engineering plant cost index (published biweekly by chemical engineering magazine),

**Note:**

In Extended cost calculations, the costs such as insurance cost, market loss cost, loss of image and prestige cost should also be considered in addition. But in this module these costs are not included.

Fig. 7. Simplified block diagram of economic module

Marshall and Swift Index (also provided in chemical engineering magazine) and Nelson-Fabaar Index (from the oil and gas journal). For the comparison of process design alternatives, these study estimates for purchased cost of process units using cost charts or equations based on them are adequate. Given the purchase cost of a process unit, the installed cost is obtained by adding the cost of installation using factored-cost methods. For each piece of equipment Guthrie (1969, 1974) provides factors to estimate the direct cost of labor, as well as, indirect costs involved in the installation procedure. The cost elements that are included in the estimation of fixed capital investment are shown in figure 8.



f.o.b ---- freight on board cost i.e. equipment purchase cost plus transport cost

Fig. 8. Typical cost elements for fixed capital investment

The operating cost (OC1) of a chemical plant is divided into two groups:

- Fixed operating cost
- Variable operating cost

The elements in fixed operating cost includes maintenance cost, operating labor cost, laboratory cost, supervision cost, plant overheads, capital charges, taxes, insurance, licence fees and royalty payments while the variable operating cost consists of raw material costs, miscellaneous operating material costs, utilities (services) and shipping and packaging. However this division of operating cost is somewhat arbitrary and depends on the accounting practice of a particular organization. The typical cost elements included in operating cost "OC1" are shown in figure 9.

However, from the existing process optimization point of view, energy cost and raw material costs are more important and often considered.

Economic module developed in this thesis using Visual basic computes fixed capital expenditure using either cost equations that have been derived by Ulrich or correlations

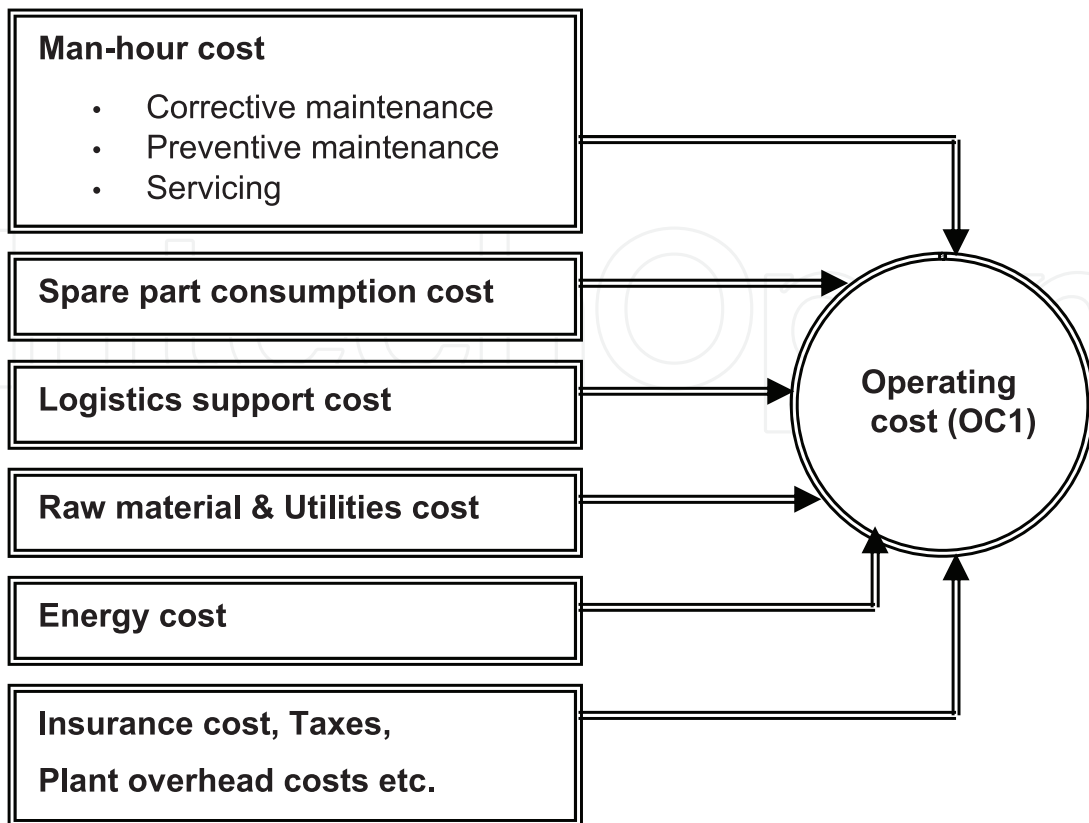


Fig. 9. Typical cost elements for operating cost (OC1)

developed by Guthrie depending on users choice, The significant operating cost for process optimization i.e. energy consumption cost (heating and cooling utilities cost) can also be calculated by using this module. Once the FCI1 and OC1 are calculated, then total annualized cost is obtained using the following equation:

$$\text{Total annualized cost (TAC1)} = d \cdot (\text{FCI1}) + \text{OC1} \quad (1)$$

Here d is depreciation or capital recovery factor and normally taken between 0.15-0.25 but can also be computed using depreciation calculation methods e.g. double declining balance method.

2.5.2 Extended cost calculations

The second section of the economic module (see Figure 7) carries out Extended cost calculations, which considers the fixed capital investment related to safety system, and risk cost due to accident and incident damage.

i. Fixed capital investment related to Safety system:

The fixed investment related to safety system is calculated by the following equation:

$$\text{FCISS} = C_{SD} + \sum_{i=1}^n N_{SE,i} \cdot C_{SE,i} \quad (2)$$

Here, the first term C_{SD} is cost for safety design (i.e. cost related to safety classification, safety requirements and design specification, detailed design and engineering, factory acceptance test or pre-start up acceptance test and start up and correction). Table 3.6 gives the typical cost elements included in C_{SD} calculations. The second term $\sum_{i=1}^n N_{SE,i} \cdot C_{SE,i}$ is the sum of the purchase cost of safety equipment. Here $C_{SE,i}$ is the purchase cost of equipment "i" and $N_{SE,i}$ is the number (count) of that equipment. The costs for these devices are based on the recent detailed survey of available costs from various suppliers conducted by Khan and Annyotte (2004), however in the module the user has the possibility to enter the present market costs.

Safety classification cost e.g SIL determination cost	C_{SIL}
Safety requirements and design specifications (SRS) cost	C_{SRS}
Detailed design and engineering cost	C_{DE}
Miscellaneous Cost:	C_{ME}
Initial training cost	C_{TC}
Factory acceptance test (FAT)/Installation/Pre-startup acceptance test (PSAT) cost	C_{FAT}
Startup and correction cost	C_{SCC}
$C_{SD} = C_{SIL} + C_{SRS} + C_{DE} + C_{ME} + C_{TC} + C_{FAT} + C_{SCC}$	

!power, wiring, junction boxes, operators interface cost

Table 6. Typical cost elements included in C_{SD} of safety system cost calculations

ii. Fixed capital investment (FCI2)

Then, extended fixed capital investment is calculated by adding FCISS to FCI1.

$$FCI2 = FCI1 + FCISS \quad (3)$$

iii. Total annualized cost (TAC2)

So, the extended total annualized cost will be calculated using extended fixed capital investment.

$$TAC2 = d \cdot (FCI2) + OC1 \quad (4)$$

Maintenance and repair cost of safety system should also be included in this calculation. But in this economic module these cost elements are not considered.

iv. Risk cost 1 (RC1)

Risk cost (RC1), which is the sum of property risk cost due to asset loss (PRC), health risk cost due to human health loss (HRC) and environmental risk cost due to environmental damage (ERC). The relations for calculation of these costs used in the module are:

Property risk cost due to asset lost (PRC) is the cost incurred due to lost of physical assets such as damage to property, loss of equipment due to accident/scenario and calculated by the equation below:

$$PRC = \sum_{i=1}^n \dot{F}_{A,i} \cdot A_{D,i} \cdot C_{A,i} \cdot t_{op} + \sum_{j=1}^n \dot{F}_{I,j} \cdot C_{D,j} \cdot t_{op} \quad (5)$$

$\dot{F}_{A,i}$ is frequency of occurring the hazardous accident, $A_{D,i}$ is damage area due to that accident, $C_{A,i}$ is the asset cost per unit area, t_{op} is total operation time, $\dot{F}_{I,j}$ is incident occurring frequency and $C_{D,j}$ is incident damage cost.

Health risk cost due to human health lost (HRC) is the cost of fatality and/or injury due to the accident scenario under study.

$$HRC = \sum_{i=1}^n \dot{F}_{A,i} \cdot N_{peop,eff} \cdot C_{H,life} \cdot t_{op} \quad (6)$$

Here, $N_{peop,eff}$ is the number of person affected due to accident and is equal to $N_{peop,eff} = pop \cdot \varphi$. Where POP is the population around the area of accident and φ is the population distribution factor (φ is 1 if population is uniform distributed (maximum value) and φ is 0.2 if population is localized and away from the area of accident (minimum value)) and $C_{H,life}$ is dollar value of human life or health. Though attempts to put value on human life have caused criticism and it changes from place to place. But a value for this can be obtained by dividing the annual gross national product by the annual number of births or by estimating how much money the person would have earned if not killed by the accident (Tweeddale 2003). A value for cost of loss of lives, marginal cost to avert the fatality, for the highest category of involuntariness risk 14×10^6 \$ is used in this work (Passman, H.J. et al. 2003).

Environmental risk cost due to environmental damage is the cost incurred due to environmental damage.

$$ERC = \sum_{i=1}^n \dot{F}_{ED} \cdot A_{ED,i} \cdot C_{ED,i} \cdot t_{op} \quad (7)$$

Where $A_{ED,i}$ is the environmental damage area due to scenario "i", \dot{F}_{ED} is the frequency of release of material to environment and $C_{ED,i}$ is the environmental damage cost per unit area.

so the sum of these three risk costs gives:

$$RC1 = PRC + HRC + ERC \quad (8)$$

v. Risk cost 2 (RC2)

Risk cost 2 (RC2), which is the sum of risk cost1 (RC1) and production loss risk cost (PLRC), accounts for accident damage risk cost. Here, production loss risk cost due to asset damage (PLRC) accounts for the cost due to the production loss because of accident and given by:

$$PLRC = \sum_{i=1}^n \dot{F}_{A,i} \cdot t_d \cdot \dot{C}_p \cdot t_{op} \quad (9)$$

Where PLRC is the production loss risk cost, t_d is the time lost due to accident and \dot{C}_p is the production loss value in \$/h. Thus Risk cost 2 (RC2) is

$$RC2 = RC1 + PLRC$$

vi. Risk cost 3 (RC3)

Risk cost 3 (RC3), which is sum of process interruption cost due the spurious trip of the safety system and process interruption cost because of safe shut down to avoid from accident, accounts for incident damage risk cost and calculated as follow:

$$RC3 = \left(\sum_{i=1}^n \dot{F}_S^{trip} \cdot t_{trip} + \dot{F}_R^{trip} \cdot t_{dR} \right) \cdot \dot{C}_p \cdot t_{op} \quad (10)$$

Here, \dot{F}_S^{trip} is spurious trip frequency, \dot{F}_R^{trip} is safe shut down frequency when trip system demand arises, t_{trip} is down time due to spurious trip and t_{dR} is down time to safe shut down when trip system demand arises.

vii. Total Risk cost (TRC)

Total Risk cost (TRC) is the sum of all risk costs:

$$TRC = RC2 + RC3 \quad (11)$$

Total risk cost can be annualized by dividing it with total operation time (t_{op}):

$$TAC_{risk} = TRC / t_{op}$$

viii. Extended Cost (ECC)

Extended cost calculations (ECC) is Life cycle related cost and calculated as follow :

$$ECC = FCI2 + PVC \quad (12)$$

Here, PVC is present value of the annual costs ($OC1, TAC_{risk}$) and calculated as follow:

$$PVC = (OC1 + TAC_{risk} - Insurance\ cost) \cdot \frac{1 - (1 + R)^{-t_{ly}}}{R}$$

R is the present interest rate and t_{ly} is the number of years (predicted life of system).

Besides, the cost elements mentioned above in Extended cost calculation section, the other elements such as warranty/insurance cost, lost of image and prestige cost, market lost cost should also be considered but quantification of these elements is still almost impossible.

2.6 Environment module

Environment module consists of four steps and introduced an environmental performance index (EPI1) for evaluation of environmental performance and environmental pollution index (EPI2) as environmental objective to be integrated along with economics. The environmental performance index (EPI1) is calculated by combining total PEI based on

WAR algorithm[16,17], resource depletion, energy conservation and fugitive emission rates while environmental pollution index (EPI2) is calculated by combining total PEI based on WAR algorithm and fugitive emissions because in this case other factors like resource depletion and energy consumption will be integrated in economic module or objective function. The Analytic hierarchy process (AHP) is used as multicriteria decision analysis tool for combining these different impacts and determination of weighting factors of individual impact categories in total PEI and later on in environmental performance index (EPI1) and environmental pollution index (EPI2) calculations. The module is developed using Microsoft Visual Basic 6.0 and WAR GUI (WAR graphical user interface) is integrated in the user plate form. The steps are:

Step I : Problem definition and data gathering

Step II : Individual impact categories calculation

Step III: Determination of weighting factors

Step IV: Environmental performance index calculation

Figure 10 shows the simplified block diagram of environment module and tasks to be performed.

2.6.1 Step I: Problem definition and data gathering

The primary task in step 1 is problem framing and scope definition. Information such as material and energy balance information, process conditions, process technology and nature of used materials/chemicals should be retrieved from process module. Process flow diagram is to be re-examined for identification of additional waste and emission streams. Collect additional data and information for environment evaluation to fill gaps. As sources of emissions such as fugitive emission sources, venting of equipment, periodic equipment cleaning, incomplete separations etc. are often missing in process so process is analyzed to identify these sources.

2.6.2 Step II: Individual impact categories calculation (Potential environmental impact calculations based on WAR algorithm)

The software WAR GUI (waste reduction algorithm graphical user interface) from the US Environmental Protection Agency is used to calculate individual potential environmental impacts. The generalized formula based on WAR algorithm for calculating individual PEI is given in equation 13.

$$PEI_L = (\dot{M}_b \cdot \sum_k^{Comps} x_{kb} \cdot \psi_{kL} + \dot{Q}_r \cdot \psi_L^E) / \dot{M}_p \quad [Impact / kg \text{ product}] \quad (13)$$

Where PEI_L is the potential environmental impact of category L, \dot{M}_b is mass flow rate of base (effluent) stream, x_{kb} is the mass fraction of component k in the base stream, ψ_{kL} is the normalized impact score of chemical k for category L, \dot{Q}_r is energy rate supplied for separation and ψ_L^E is the normalized impact score of category L due to energy. The sensitivity analysis results of individual potential environmental impact with respect to optimization variables should also be performed.

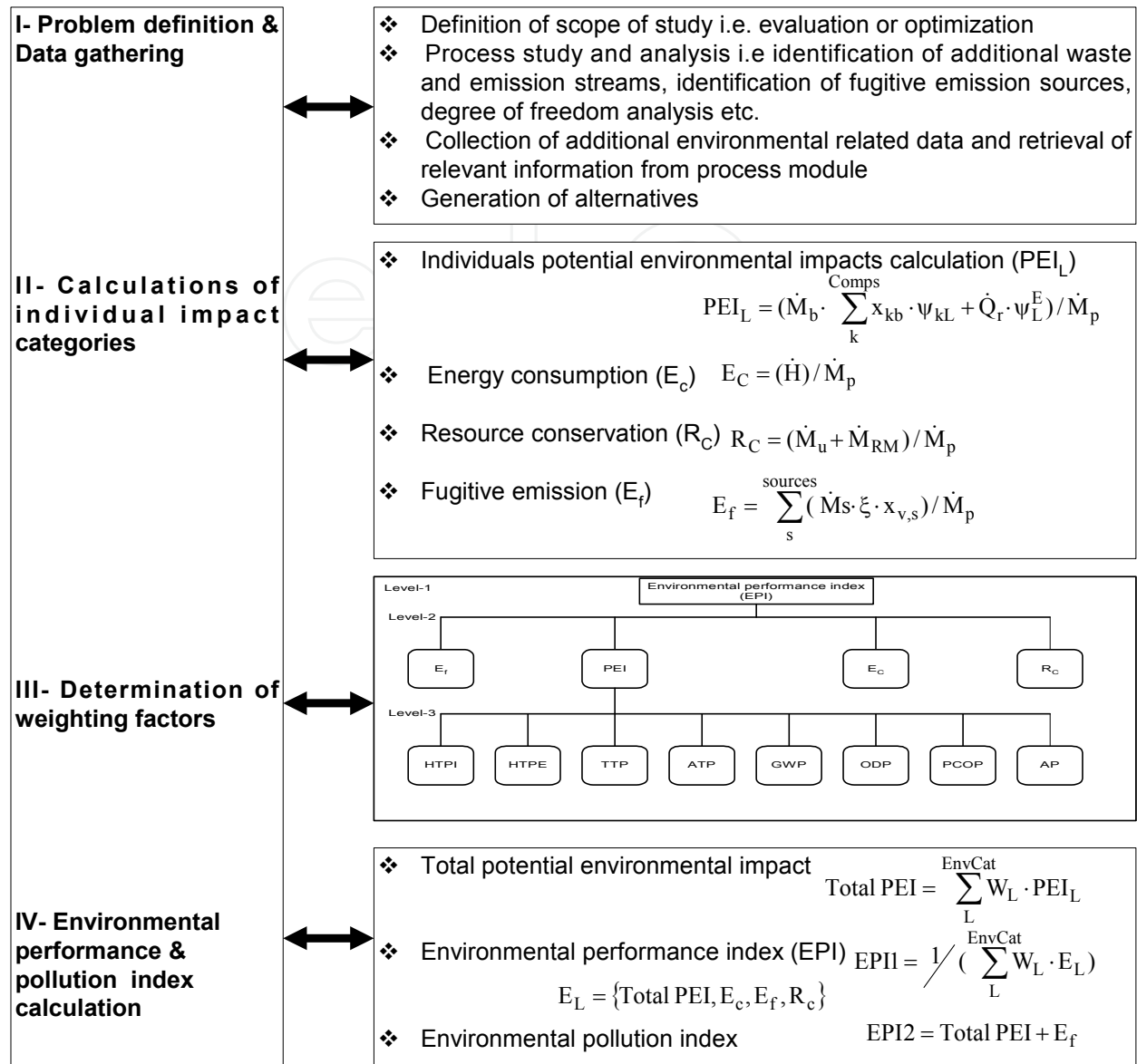


Fig. 10. Simplified block diagram of environment module

Energy consumption factor (E_C)

Energy consumption factor refers the total amount of energy consumed in the process per unit of product and is calculated as follow:

$$E_C = (\dot{H}) / \dot{M}_p \quad [kJ / kg\ product] \quad (14)$$

Here $\dot{H} = \dot{M}_{steam} \cdot \hat{h}_{steam} + E_E$ where \dot{M}_{steam} is the mass flow rate of steam [kg/h], \hat{h}_{steam} is the enthalpy of steam per kg [KJ/kg], E_E is electrical energy consumed per unit time [KJ / h] and \dot{M}_p is product rate [kg/h].

The sensitivity analysis of this factor with respect to optimization variables should also be performed.

Resource conservation factor (R_C)

The resource consumption refers all needed raw materials and utilities used and given by:

$$R_C = (\dot{M}_u + \dot{M}_{RM}) / \dot{M}_p \quad [\text{kg} / \text{kg product}] \quad (15)$$

Where R_C is the resource conservation factor, \dot{M}_u is utilities consumption rate, \dot{M}_{RM} is raw material consumption rate.

Fugitive emission factor (E_f)

Fugitive emissions are unplanned or unmanaged, continuous or intermittent releases from unsealed sources such as storage tank vents, valves, pump seals, flanges, compressors, sampling connections, open ended lines etc and any other non point air emissions. These sources are large in number and difficult to identify. These emission rates depends on factors such as the age and quality of components, specific inspection and maintenance procedures, equipment design and standards of installation, specific process temperatures and pressures, number and type of sources and operational management commitment[18]. However, four basic approaches for estimating emissions from equipment leaks in a specific processing unit, in order of increasing refinement, in use are:

- Average emission factor approach
- Screening ranges approach
- EPA correlation approach
- Unit-specific correlation approach

All these approaches require some data collection, data analysis and/or statistical evaluation. On the other hand, using fundamental design / engineering calculations for accurate fugitive emission estimations for each source present in the process industry are difficult due to:

- large number and type of fugitive emission sources
- dependence of emission rates on other factors along with design and operating conditions e.g. installation standards, inspection and maintenance procedure etc.

As focus in this work is to integrate fugitive emissions into environmental performance evaluation and optimization objectives so average emission factor approach giving a bit over estimates are used. Average emission factors for estimating fugitive emissions from fugitive sources found in synthetic organic chemical manufacturing industries operations (SOCMI) obtained from the US Environmental Protection Agency L & E Databases are used. The relation used in this work for calculation of fugitive emissions is:

$$E_f = \sum_s^{\text{sources}} (\dot{M}_s \cdot \xi \cdot x_{v,s}) / \dot{M}_p \quad [\text{kg} / \text{kg product}] \quad (16)$$

Here E_f is fugitive emission factor per unit of product, \dot{M}_s mass flow rate through the source 's', ξ is average emission factor and $x_{v,s}$ is mass fraction of volatile component through source 's' and \dot{M}_p is product rate. It is assumed $x_{v,s}$ for the process fluids through

fugitive sources such as pump seals, valves, flanges and connection is equal to 1, i.e. fluids are composed entirely of volatile compounds.

2.6.3 Step III: Determination of weighting factors (Application of multicriteria decision analysis technique)

The integration of these individual impact categories into one index is a hierarchical multicriteria decision analysis problem. The analytic hierarchy process (AHP) is used for this purpose[19] and a computer programme for it is developed in VB 6.0. In this stage, first a hierarchical structure of the problem, which is structured hierarchically similar to a flow chart, is constructed. The overall objective is placed at the top while the criteria and sub-criteria are placed below. For example, as shown in figure 11, the overall objective Environmental performance index (EPI1) is placed at the top (level 1), then below (level 2) are criterias Total PEI, E_f , E_c and R_c and after this (level 3) sub-criterias as HTPI, HTPE, TTP, ATP, GWP, ODP, PCOP and AP. After this using the numerical scale given in table 2.6, two pairwise comparison matrices (see Table 7 and 8) are constructed for determination of weights for aggregation of individual impact categories of WAR to total PEI and for determination of weights of total PEI, E_f , E_c and R_c to Environmental performance index (EPI1).

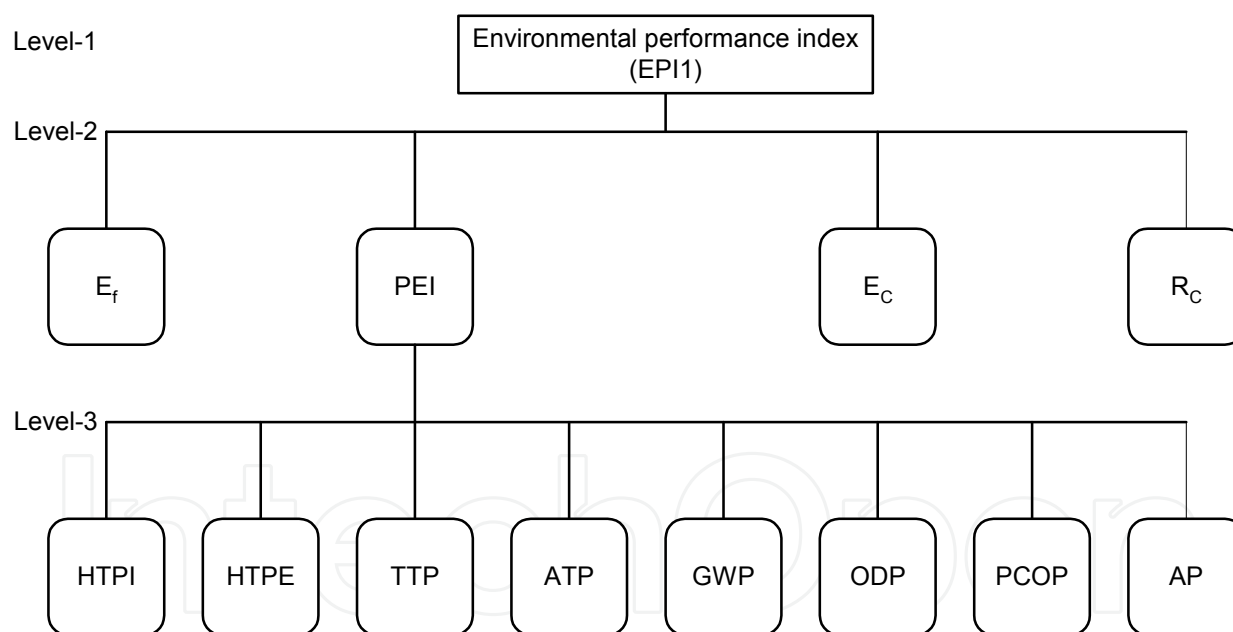


Fig. 11. Hierarchical structuring of multicriteria decision analysis problem for integrating individual environmental impacts

The right hand upper diagonal information in both matrices is to be provided by the decision maker giving the relative importance of the two criteria using the numerical scale of table 2.6 while the left hand lower diagonal is the reciprocal of the right hand upper diagonal. Once these pair wise comparison matrices are constructed, then developed computer programme using the AHP method, determines the weighting of individual impact categories. The level of inconsistency of decision makers input is checked by

Pairwise comparison matrix								
	HTPI	HTPE	TTP	ATP	GWP	ODP	PCOP	AP
HTPI	1	A12	A13	A14	A15	A16	A17	A18
HTPE		1	A23	A24	A25	A26	A27	A28
TTP			1	A34	A35	A36	A37	A38
ATP				1	A45	A46	A47	A48
GWP					1	A56	A57	A58
ODP						1	A67	A68
PCOP							1	A78
AP								1
W _L	W1	W2	W3	W4	W5	W6	W7	W8

Table 7. Pairwise comparison matrix for individual impact categories at level 3

Pairwise comparison matrix				
	PEI	R _C	E _C	E _f
PEI	1	A12	A13	A14
R _C		1	A23	A24
E _C			1	A34
E _f				1
W _L	W1	W2	W3	W4

Table 8. Pairwise comparison matrix for individual impact categories at level 2

consistency ratio before giving the output. Consistency ratio less than 0.1 is good and for ratios greater than 0.1, the input to pair wise matrix should be re-evaluated.

2.6.4 Step IV: Environmental performance & pollution index calculation

In the final step, first Total PEI is determined by multiplying each impact category values with its relevant weighting factor W_L as given below:

$$Total\ PEI = \sum_L^{EnvCat} W_L \cdot PEI_L \quad (17)$$

After calculating Total PEI, Environmental performance index (EPI1) is determined for each alternative by multiplying the values of Total PEI, E_f, E_C and R_C with its relevant weighting factor W_L (table 8) as given below:

$$EPI1 = 1 / \left(\sum_L^{EnvCat} W_L \cdot E_L \right) \quad (18)$$

Where $E_L = \{Total\ PEI, E_c, E_f, R_c\}$

and environmental pollution index (EPI2) is calculated as follow

$$EPI2 = Total\ PEI + E_f \quad (19)$$

The higher value of environmental performance index (EPI1) shows that the process is environmentally better and vice versa. While the higher value of environmental pollution index (EPI2) shows that the environmental performance of process is worse.

2.7 Data manager

The relevant information generated from process module, safety module and environment module for each alternative is transferred to data manager. This information is used to formulate process diagnostic tables and multiobjective decision-making problem formulation. These tables consist of mass input/output table, energy input/output table, capital and utility annual expense summary, environmental impact summary and frequency of occurrence of an event and their consequence categories and safety cost.

2.8 Stage III: Multiobjective decision analysis/ optimization

The purpose of this layer/stage is to set up multiobjective decision making/optimization among these conflicting objectives. The aim is to find out the trade-off surface for each alternative and /or complete ranking of alternatives. The calculation loop used for it is shown in figure 12.

In each independent performance module i.e. economic, environment and safety module, relevant information is generated and transferred automatically or manually to data manager for each alternative generated or under study. Before transferring the values of performance objective functions, each objective function is optimized within their independent module such as:

- Process/Economic optimization of each alternative is carried out using SQP optimization algorithm build within Aspen Plus™.
- The lower and upper limits for Environmental objective functions are calculated using environmental module from the material and energy balance information from process model.
- Safety/risk aspects are optimized in the safety module and information such as hazard occurrence frequency, safety cost data (fixed safety system cost, accident and/or incident damage risk cost) for each alternative is transferred to the data manger.

Depending on the case under study or objectives of the study, graphical tool box of MatLab and/or multiobjective optimization technique (goal programming) or multiattribute decision analysis technique (PROMETHEE and/or AHP) is used for multiobjective decision analysis. The Data Manager is linked with MatLab 7.0 via Excel link Toolbox in the

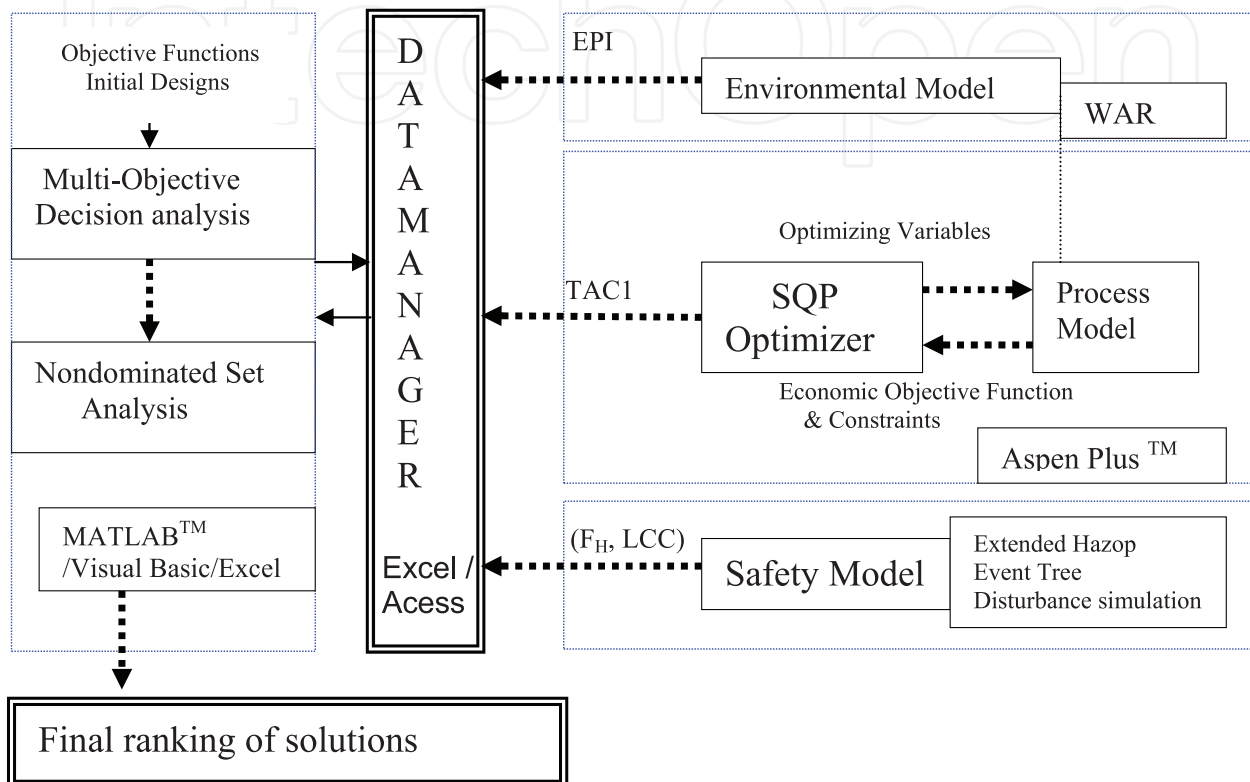


Fig. 12. Calculation loop for multiobjective optimization

integrated interface. Aspen plusTM is linked in the integrated interface via Visual basic 6.0 and Microsoft Excel. AHP technique is also programmed for the cases under study in Visual basic 6.0. The computer realization of these links in the integrated interface is explained in chapter four.

2.9 Stage IV: Design evaluation

The purpose of this layer/stage is to select the best alternative and/or find the complete ranking of alternatives under study based on the results of third stage/layer of the developed methodology. Pareto approach (non dominated analysis) or PROMETHEE is used for this purpose.

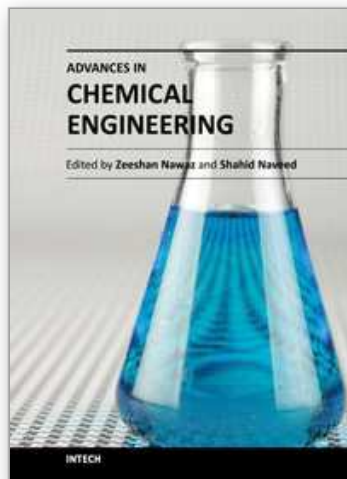
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Chemical engineering applications have been a source of challenging optimization problems in terms of economics and technology. The goal of this book is to enable the reader to get instant information on fundamentals and advancements in chemical engineering. This book addresses ongoing evolutions of chemical engineering and provides overview to the state of the art advancements. Molecular perspective is increasingly important in the refinement of kinetic and thermodynamic modeling. As a result, much of the material was revised on industrial problems and their sophisticated solutions from known scientists around the world. These issues were divided into two sections, fundamental advances and catalysis and reaction engineering. A distinct feature of this text continues to be the emphasis on molecular chemistry, reaction engineering and modeling to achieve rational and robust industrial design. Our perspective is that this background must be made available to undergraduate, graduate and professionals in an integrated manner.

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