CHAPTER II

BACKGROUND AND LITERATURE SURVEY

2.1 Environmental Impact

In this work, an indicator quantifying environmental impact is the environmental impact index of each chemical. Based on the work by Young and Cabezas, (1999); Dantus and High, (1999).

2.1.1 Calculation of Environmental Impact Units

Environmental Impact Units (EIU) per kilogram of product (Dantus & High, 1999) produced

$$\theta = \frac{\sum_{i=1}^{n}\sum_{k=1}^{m} w_i m_{k,i} \Psi_k}{P} \tag{2.1}$$

where

θ = Environmental impact (EIU/kg)

w_i = Flowrate of waste stream k (kg/h)

P = Product flowrate (kg/h)

Ψ_k = Environmental impact index of chemical k (EIU/kg)

$m_{k,i}$ = Mass fraction of component k in waste stream i

Environmental impact index of chemical k (Young & Cabezas, 1999)

$$\Psi_k = \sum_l \alpha_l \Psi_{kl}^s \tag{2.2}$$

where

$$\Psi_{kl}^s = \frac{(Score)_{kl}}{\langle (Score)_k \rangle_l}$$

α_l = the relative weighting factor of impact category l

(ranged between 0 and 10)

$(Score)_{kl}$ = the value of chemical k on some arbitrary scale for category l

$\langle (Score)_k \rangle_l$ = the average value of all chemicals in category l

The classification of impact categories fall into 2 general areas (Young and Cabezas, 1999) of concern with four categories in each area: global atmospheric and local toxicological.

Global atmospheric impact categories

1. Global warming potential (GWP)
2. Ozone depletion potential (ODP)
3. Acidification or acid-rain potential (AP)
4. Photochemical oxidation or smog formation potential (PCOP)

Local toxicological impact categories

1. Human toxicity potential by ingestion (HTPI)

$$(Score)_{k,HTPI} = \frac{1}{(LD_{50})_k} \tag{2.3}$$

2. Human toxicity potential be either inhalation or dermal exposure (HTPE)

$$(Score)_{k,HTPE} = \frac{1}{(TLV)_k} \tag{2.4}$$

3. Aquatic toxicity potential (ATP)

$$(Score)_{k,ATP} = \frac{1}{(LD_{fish50})_k} \tag{2.5}$$

4. Terrestrial toxicity potential (TTP)

$$(Score)_{k,TTP} = \frac{1}{(LD_{50})_k} \tag{2.6}$$

where

LD_{50}= The lethal-dose that produced death in 50% of rats by oral ingestion.

TLV= Threshold limit value which is the concentration limit for individual exposures in the workplace environmental.

LC_{fish50}= a lethal concentration which causes death in 50% of the test specimens (fish).

2.2 Economic Analysis

2.2.1 Estimation of Total Capital Investment

Method: Percentage of Delivered-equipment Cost (Peters *et al*, 2003) is introduced to estimate capital investment requiring determination of the delivered-equipment cost. The other items included in the total direct and indirect plant costs, or total capital investment are estimated as percentages of the delivered-equipment cost. The cost equation summarizes this method as

$$C_n = \sum E(1 + f_1 + + f_2 + f_3 + \ldots + f_n) \quad (2.7)$$

where

E = Purchased-equipment cost on f.o.b. basis, dollars.

$f_1, f_2, f_3, \ldots, f_n$ = multiplying factors purchased-equipment installation instrumentation and controls, indirect cost, etc.

The factors used in making estimation are determined on the basis of the types of process plants which fluid processing plant is used as a basis. Table 2.1 for fluid processing plant shows the predesign estimate for capital investment costs.

Estimating by the method is normally used for preliminary and study estimates that the uncertainty is approximations with ±20 to 30%, thus assuming the total capital investment is equal to 30% uncertainty.

Table 2.1 Ratio factors for estimating capital investment items based on delivered-equipment cost

	Percent of delivered-equipment cost for fluid processing plant
Direct Costs	
Purchased equipment delivered	100
Purchased equipment installation	47
Instrumentation & Controls(installed)	36
Piping (installed)	68
Electrical systems (installed)	11
Buildings (including services)	18
Yard improvements	10
Service facilities (installed)	70
Total direct costs	360
Indirect Costs	
Engineering and supervision	33
Construction expenses	41
Legal expenses	4
Contractor's fee	22
Contingency	44
Total indirect costs	144
Fixed capital investment (FCI)	504
Working capital (WC)	89
Total capital investment (TCI)	**593**

2.2.2 Estimation of Total Product Cost

The total production cost can be divided into two categories: manufacturing cost (operation or production cost) and general expenses. The manufacturing costs compose of variable production cost, fixed charges, and plant overhead costs. Table 2.2 summarizes the predesign estimate for total product costs.

Table 2.2 Estimation of total product cost

Manufacturing Cost	**Assumption**
A. Direct production costs	
1 Raw materials	
2 Operating labor	
3 Operating supervision	0.15 of operating labor
4 Utilities	
5 Maintenance and repairs	0.06 of FCI
6 Operating supplies	0.15 of maintenance & repair
7 Laboratory charges	0.15 of operating labor
8 Catalysts and solvents	
B. Fixed charges	
1 Taxes (property)	0.02 of FCI
2 Financing (interest)	0 of FCI
3 Insurance	0.01 of FCI
4 Rent	
5 Depreciation	MACRS 5-year
C. Plant overhead cost	0.6 of labor, supervision and maintenance
General Expenses	**Assumption**
A. Administration	0.2 of labor, supervision and maintenance
B. Distribution & selling	0.05 of c_o
C. Research & Development	0.04 of c_o
Total Product Cost (c_o)	Manufacturing Cost + General Expenses

2.2.3 Methods for Calculating Profitability

Analyzing the profitability, the rate of return on investment (ROI) and the net present worth (NPW) is used as tools.

Net Present Worth (NPW) This profitability measure is defined as the total of the present worth of all cash flows minus the present worth of all capital investment. This can be expressed as

$$NPW = \sum PWF_{cf,j}\left[\left(s_j - c_{oj} - d_j\right)\left(1-\Phi\right) + rec_j + d_j\right] - PWF_{v,j}T_j \qquad (2.8)$$

where NPW = the net present worth

PWF_{cfj} = the selected present worth factor for the cash flow in year j

s_j = the value of sales in year j

c_{oj} = the total product cost not including depreciation in year j

d_j = depreciation charge in year j, dollars

PWF_{vj} = the worth factor for investments occurring in year j

T_j = total capital investment in year j

rec_j = recovery of working capital and physical asserts in year j, dollars

Φ = income tax rate, percent/100

2.3 Environmental Impact and Uncertainty

The uncertainty of harmful environmental impact could be directly attributed to the uncertainty in the parameters which is used in the design. The conditions lead to variable impact throughout time are considered and varied. The environment conditions used to calculate the indices and possibly other factors as market conditions, which lead to different operating conditions of the designed plant. In addition, uncertainties can also arise from the fact that human health effects or other similar parameters used in the calculation of the indices are also uncertain in nature, but considered as fixed numbers in the indicators.

A classical single criteria design paradigm shown below is dominated by the cost. Although risk can be defined in a probabilistic sense, and even calculated a-posteriori, risk is not managed in any proper work.

Minimize {Expected Cost}
Subject to
Material and Energy balances
Property calculation equations
Equipment design equations
Containment of expected values of environmental impact
Containment of risk (environmental and financial)
(2.9)

The below is a multicriteria optimization formulation which is a methodology to address design under uncertainty that is used to manage both of the risks (environmental and financial), an expected cost, and expected environmental impact index, simultaneously.

$$\left.\begin{array}{l}\text{Minimize \{Expected Cost, Expected Environmental Impact Index,}\\ \qquad\qquad\text{Risks (both)\}}\\ \text{Subject to}\\ \text{Material and Energy balances}\\ \text{Property calculation equations}\\ \text{Equipment design equations}\end{array}\right\} \quad (2.10)$$

Without the use of risk, this is the formulation suggested by Dantus and High (1999).

2.4 Background on Two-Stage Decision Making Stochastic Models

The two-stage decision making stochastic models (Barbaro and Bagajewicz, 2003) can be divided into two essential features. The first is called the *first-stage decisions* or *here and now decisions* and the other is the *second-stage decisions* or *recourse decisions*. The *first-stage decisions* taken at the planning time, that is, before the uncertainty is discovered such as capital investment. At a later time, the decisions made after knowing the uncertainty is the second-stage decisions which is often operational. Planning process capacity expansions under uncertainty are one type of systems widely studied using these techniques (Sahinidis *et al.*, 1989; Liu and Sahinidis, 1996).

The general extensive form of a two-stage mixed-integer linear stochastic problem with fixed recourse and a finite number of scenarios is:

Model SP: $Max \ E[Profit] = \sum_{s \in S} p_s q_s^T y_s$ (2.11)

Subject to

$Ax = b$ (2.12)

$c_1^T x + c_2^T y_s < C$ (2.13)

$T_s x + W y_s = h_s \quad \forall s \in S$ (2.14)

In the above model, x represents the first-stage mixed-integer decision variables and y_s are the second-stage variables corresponding to scenario s, which has probability

p_s. The uncertain parameters in this model appear in the coefficients q_s, the matrix T_s, and in the independent terms h_s. We are restricted to the cases where W, the recourse matrix, is fixed. This assures that the second-stage feasible region is convex and closed, and that the recourse function is a piecewise linear convex function in x. Extensions to the nonlinear cases, which constitute our problem, are straightforward. We concentrate on the issue of risk next.

2.5 Risk

The variability of the profit over the different scenarios cannot be provided by using Model SP. For example, consider the histogram of two feasible solutions of a project shown in Figure 2.1 (Barbaro and Bagajewicz, 2003).

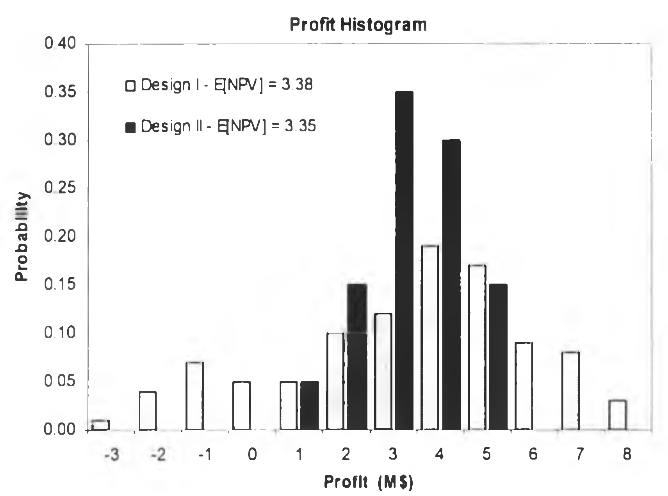

Figure 2.1 Profit histogram for two cases of resource allocation.

The first design has a larger expected profit (3.38) than the second (3.35); however, Design I is riskier than Design II. If one defines risk as the probability of profit to be smaller than a certain number, then one can conclude that Design I contains several scenarios where a small profit is expected, whereas Design II has no scenario where loss is expected. Thus, a risk-averse decision maker would prefer Case II, but all this depends on the profit expectation level chosen. For example, if risk is now thought of as the probability of having a profit of 7 or more, then Case II is riskier. However, a risk-averse decision maker will always prefer to look at the lower value of profit target than at a larger one. Thus, this kind of preferences cannot be captured by using the model SP. So, a proper measure of financial risk needs to be integrated to allow the decision maker to achieve solutions of his/her desired risk exposure level.

Under uncertainty, risk is defined as the probability of not meeting a certain target objective function level referred to as Ω. The risk associated with a design x and a target Ω is therefore expressed by the following probability (Figure 2.2):

$$Financial\_Risk(x,\Omega) = P(Profit(x) < \Omega) \tag{2.15}$$

where Profit(x) is the actual profit, i.e., the profit resulting after the uncertainty has been uncovered and a scenario realized. Since profit can be related to a summation over a set of independent scenarios, we have

$$Financial\_Risk(x,\Omega) = \sum_{s \in S} p_s \, z_s(x,\Omega) \tag{2.16}$$

where z_s is a new binary variable defined for each scenario, that takes the value of 1, when $Profit_s(x) < \Omega$, and zero otherwise A way of a assessing and understanding the trade-offs between risk and profit is to use the cumulative risk curve, as depicted in Figure 2.3 for the continuous case (Barbaro and Bagajewicz, 2003), which is the limit for a large number of scenarios.

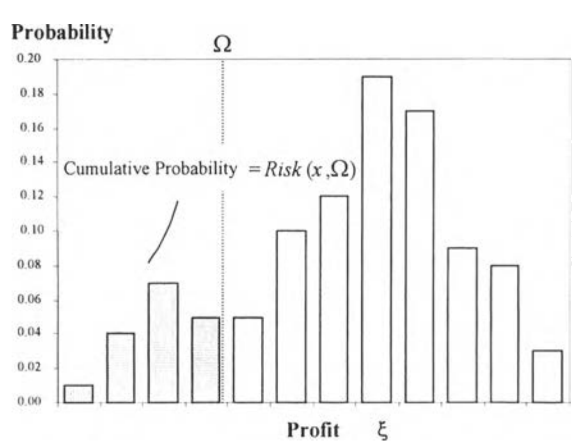

Figure 2.2 Definition of risk. Discrete Case.

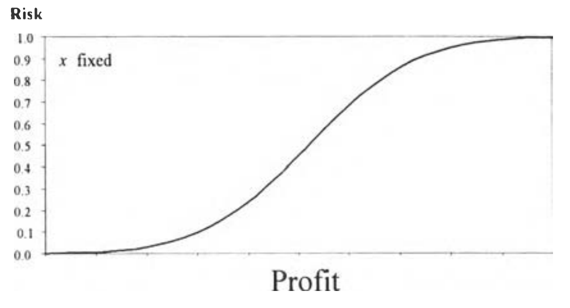

Figure 2.3 Risk curve. Continuous case.

Management of the shape and position of the curve is the main interests of the decision maker. Figure 2.4 illustrates a hypothetical example with two types of risk curves that a risk-averse decision maker may want to have low risk for some conservative low aspiration level, while a risk-taker one would prefer to see lower risk at higher aspiration level, even if the risk at lower target values increases. Another very important result that Barbaro and Bagajewicz (2003) proved formally is that no feasible design x has a risk curve that lies entirely beneath the curve depicting risk of the optimal solution to problem SP and both risk curves either cross at some point(s) (as in Figure 2.4) or the latter lies entirely above (below) the former.

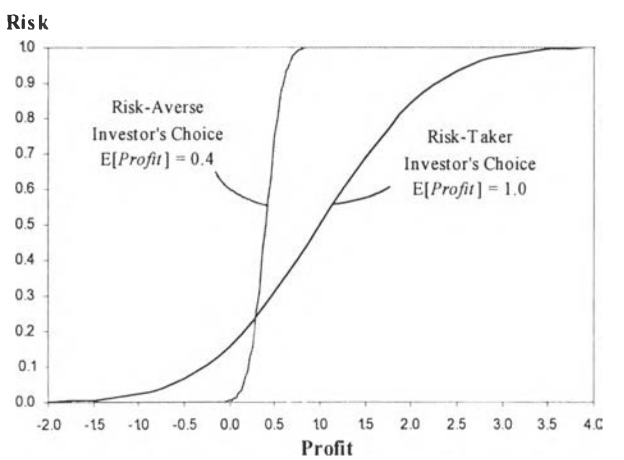

Figure 2.4 Different kinds of risk curves.

2.5.1 Managing Risk at the Design Stage

A decision maker requests to maximize the expected profit and minimize the risk at every level at the same time, which may appear as a two-objective trade-off, however, it is interesting that a solution that minimizes risk at every target also maximize the expected net present value. Thus, minimizing $Risk(x,\Omega)\ \forall\Omega\in\Re$ and maximizing $E[Profit(x)]$ are equivalent objectives. However, minimizing risk at some levels has a trade off with expected profit. As the mentioned above, a risk-averse decision maker will feel comfortable with low risk at low values of Ω. However, the price to pay is that minimizing the risk at low values of Ω conflicts with minimizing the risk at high values of Ω and vice versa. In turn, minimizing $Risk(x,\Omega)$ for a continuous range of targets Ω results in an infinite multi-objective optimization problem, which can be approximated by a finite multi-objective problem that only minimizes risk at some finite number of targets and maximizes profit, as shown in Figure 2.5.

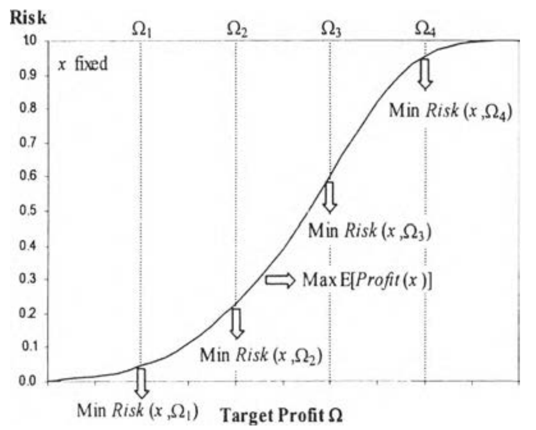

Figure 2.5 Multiobjective approach.

Figure 2.6 depicts a set of hypothetical solutions to illustrate the usefulness of the above multi-objective formulation. Solutions 2 and 3 maximize the expected profit with minimum financial risk at targets Ω_2 and Ω_1, respectively. Thus, minimizing risk at each target independently of other targets results in designs that perform well around the specific target but do poorly in the rest of the range. When risk, on the other hand, is minimized for every target at the same time, solutions that perform well in the entire range of interest may be found. Barbaro and Bagajewicz (2003) proposed a multiobjective methodology to generate all these curves.

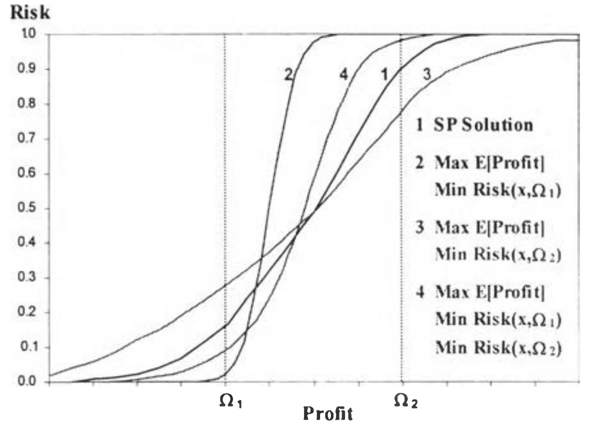

Figure 2.6 Spectrum of solutions.

The formulations developed by Barbaro and Bagajewicz (2003) address the problem of controlling the risk curve in order to get solutions that satisfy the decision maker's criteria.

2.6 Multiobjective Optimization

In the presence of more than one objective, that are conflicting each other, so the multiobjective optimization is introduced to produce optimal solutions under some specified criteria. The optimum solution obtained will be considered as the best compromise solution, which is dealing with several objectives there is usually no alternative that maximizes or minimizes each criterion simultaneously.

Applying the compromise programming approach, the four-objective optimization used to evaluate design is given by

$$\min L_{j,i} = \begin{array}{l} \gamma_{NPW}\left(\dfrac{E(NPW_{\max}) - E(NPW(x,y))}{E(NPW_{\max}) - E(NPW_{\min})}\right)^{j} - \gamma_{EI}\left(\dfrac{E(EI_{\min}) - E(EI(x,y))}{E(EI_{\max}) - E(EI_{\min})}\right)^{j} + \\ \gamma_{NPW,i}\left(\dfrac{NPW_{\max,i} - NPW(x,y)_{i}}{NPW_{\max,i} - NPW_{\min,i}}\right)^{j} - \gamma_{EI,i}\left(\dfrac{EI_{\min,i} - EI(x,y)_{i}}{EI_{\max,i} - EI_{\min,i}}\right)^{j} \end{array} \qquad (2.17)$$

subject to: $g(x,y) = 0$

$h(x,y) \leq 0$

where, $E(x)$ = Expected value of x

$NPW_{\max,i}$	=	Max NPW(x,y) at risk of i
$NPW(x,y)_i$	=	NPW(x,y) at risk of i
$NPW_{\min,i}$	=	Min NPW(x,y) at risk of i
$EI_{\min,i}$	=	Min EI(x,y) at risk of i
$EI(x,y)_i$	=	EI(x,y) at risk of i
$EI_{\max,i}$	=	Max EI(x,y) at risk of i
γ	=	Preference weight
L_j	=	Distance from the ideal point at risk of i
g( )	=	Set of equality constraints
h( )	=	Set of inequality constraints
x	=	vector of continuous variables
y	=	vector of discrete variables

The four-objective optimization is used to maximize E(NPW), minimizing E(EI), maximize NPW and minimize EI at risk i which is an interested or accepted risk point for a decision-maker. Risk curves (see Figure 2.3) is used to determined NPW(x,y) and EI(x,y) at risk of i.