Published, Resources, Conservation, and Recycling, 44(2005), 215-235. (Invited Paper)

DTD 5

ARTICLE IN PRESS

ELSEVIER

Available online at www.sciencedirect.com

SCIENCE DIRECT®

Resources, Conservation and Recycling xxx (2005) xxx–xxx

Resources Conservation & Recycling

www.elsevier.com/locate/resconrec

Green process design, industrial ecology, and sustainability: A systems analysis perspective

Urmila Diwekar *

Department of Bio, Chemical, and Industrial Engineering and Institute for Environmental Science and Policy, University of Illinois at Chicago, MC-063, Chicago, IL 60607, USA

Accepted 18 January 2005

Abstract

This paper presents a systems analysis perspective that extends the traditional process design framework to green process design and industrial ecology leading to sustainability. For green process design this involves starting the design decisions as early as chemical and material selection stage on one end, and managing and planning decisions at the other end. However, uncertainties and multiple and conflicting objectives are inherent in such a design process. Uncertainties increase further in industrial ecology. Combining AI approaches with optimization methods, and constraining the system using thermodynamics and physics can provide a way to address this problem. The concept of overall sustainability goes beyond industrial ecology and brings in time dependent nature of the ecosystem and multi-disciplinary decision making. Optimal control methods and theories from financial literature can be useful in handling the time dependent uncertainties in this problem.

Keywords: Sustainability; Process design; Industrial ecology; Optimisation; Multi-objective; Uncertainty analysis; Systems analysis; Options theory; Ito processes

1. Introduction

Computer aided simulation models and other design tools allow engineers to design, simulate, and optimize chemical processes. However, there is a critical need to incorpo-

* Tel.: +1 312 355 3277; fax: +1 312 996 5921.
E-mail address: urmila@uic.edu.

0921-3449/$ – see front matter
doi:10.1016/j.resconrec.2005.01.007

rate green engineering into the design of these processes (Diwekar, 2003a). This calls for extending the breadth of the design process to incorporate ecological and sustainability issues early in design. This paper presents a systems analysis perspective for extending the traditional design framework from green process design, to industrial ecology, to sustainability. As a first step, the framework extends the traditional design framework to include decisions starting from chemical and material selection, to management and planning. This integration poses challenging problem of discrete and continuous decisions, and nonlinear models. As the envelope is extended, the uncertainties in the model increase. Further, green engineering concepts change the single goal of engineering design from profitability to include number of different and conflicting objectives that can define the sustainability in the end.

In industrial ecology, this decision making changes from the small scale of a single unit operation or industrial production plant to the larger scales of an integrated industrial park, community, firm or sector, the available management options expand from simple changes in process operation and inputs to more complex resource management strategies, including integrated waste recycling and reuse options. The concept of overall sustainability goes beyond industrial ecology and brings in time dependent nature of the ecosystem. Decisions regarding regulations, human interactions with ecosystem come in picture. It involves dealing with various time scales and time dependent uncertainties which require appropriately modeling these. The activity is data intensive, however, mass and energy balance, and thermodynamic principles can be utilized to identify, predict, and bridge the data gaps. Further, sophisticated system analysis tools based on efficient optimization, artificial intelligence (AI) algorithms, and methods for uncertainty analysis can provide a plausible option to address this Herculean task. This paper outlines the approach in following sections. Section 2 describes the systems approach to green process design followed by Section 3 on Industrial ecology leading to Section 4 on overall Sustainability. Finally, Section 5 concludes the paper with a summary.

2. Green process design

Process simulation is defined as the utilization of computer software resources to develop mathematical models for the construction of an accurate, representative model of a chemical process in order to understand its actual behavior during regular plant operations. Steady state simulators like PRO-II, ASPEN Plus (Aspen tech, 2003a) are well known in this area and are extensively used for simulation of continuous chemical processes. Although batch process simulators are not yet reached the same maturity due to the complexities associated with the unsteady state and flexible nature of batch processing, they have become more sophisticated over the years (Aspen tech, 2003b; Shanklin et al., 2001; Diwekar, 1996). Chemical process industries have become aware of the importance of reducing waste and these industries are practicing the art of pollution prevention. These trends are also reflected in these simulation packages. In the past, process simulation was mainly concerned with the development of sophisticated unit operation blocks to predict accurate mass flows of principal components in a process. In recent years, environmental consciousness and considerations in chemical process design and simulation demand an effort extending far beyond the capability of existing process simulators to model processes with environmental control options. For tracking of trace components and demands non-equilibrium based models are provided. Packages like the waste reduction algorithm (WAR) (EPA, 2002) provides data related to various environmental impacts like toxicity and exposure data and existing simulators are equipped with thermodynamic models to characterize the impacts (e.g. infinite dilution activity coefficients for solvent selection). Group contribution methods to facilitate molecular design level synthesis are also available now (Molecular Knowlege Systems, 1994, 1998). However, there is still a long way to attain the goal of sustainability. Recently, Anastas and Zimmerman (2003) presented twelve principles of green engineering to achieve sustainability through science and technology. For example, currently, environmentally friendly or "green" processes are designed based on concepts of process integration, which embodies a number of closely-related methodologies for designing new processes and retrofitting existing ones by taking into consideration the performance of the entire process as a whole (Rossiter, 1994; Ei-Halwagi, 1997). The main advantage of process integration is that it is inherently "conservation oriented" and enhance the process performance by minimizing the use and/or maximizing the recovery of energy and materials. In addition to process integration, integrated environmental control strategies introduced in the early design stages of a process, rather than an end-of-pipe control option introduced in the later stages, have been shown to improve the technical and economic performance of a process. However, to attain sustainability one has to extend this framework beyond process integration and environmental control technologies. This means introducing green engineering principles as early as possible, and at all levels of engineering decision making. However, integrating all these principles at all levels is an onerous task. Fig. 1 shows the integrated framework proposed by the author (Diwekar, 2003a) to include the green engineering principles at all stages. Unlike the traditional process design where engineers are looking for low cost options, environmental considerations include various objectives like the long term and short-term environmental and other impacts. This new framework includes decisions at all levels starting from the chemical or material selection to the process synthesis stages, to the management and planning stage, linked to the green objectives and goals shown on the top left left-hand corner of the figure.

Fig. 1 shows that the decision making is driven by objectives such as costs, environmental impacts, reliability etc. However, this requires the ability to model the phenomena and to include uncertainties in predicting the various objectives. This is particularly important for new environmental friendly technologies like the fuel cell technology for power generation. The next subsection presents the importance of uncertainty analysis in obtaining greener and environmentally friendly plants for energy generation.

2.1. Multi-objective designs for a hybrid fuel cell power plant under uncertainty

As the first step towards a multi-objective analysis for obtaining cleaner, efficient, cost-effective and greener electricity, a fuel cell hybrid plant design case study is presented here. The study, which is sponsored by the National Energy Technology Laboratories (NETL), is based on a hybrid fuel cell power plant system that uses both solid oxide fuel cells (SOFC) as well as polymer electrolyte fuel cells (PEM). The aim of case study is to illustrate the benefits of using the multi-objective optimization methods to obtain designs with minimum

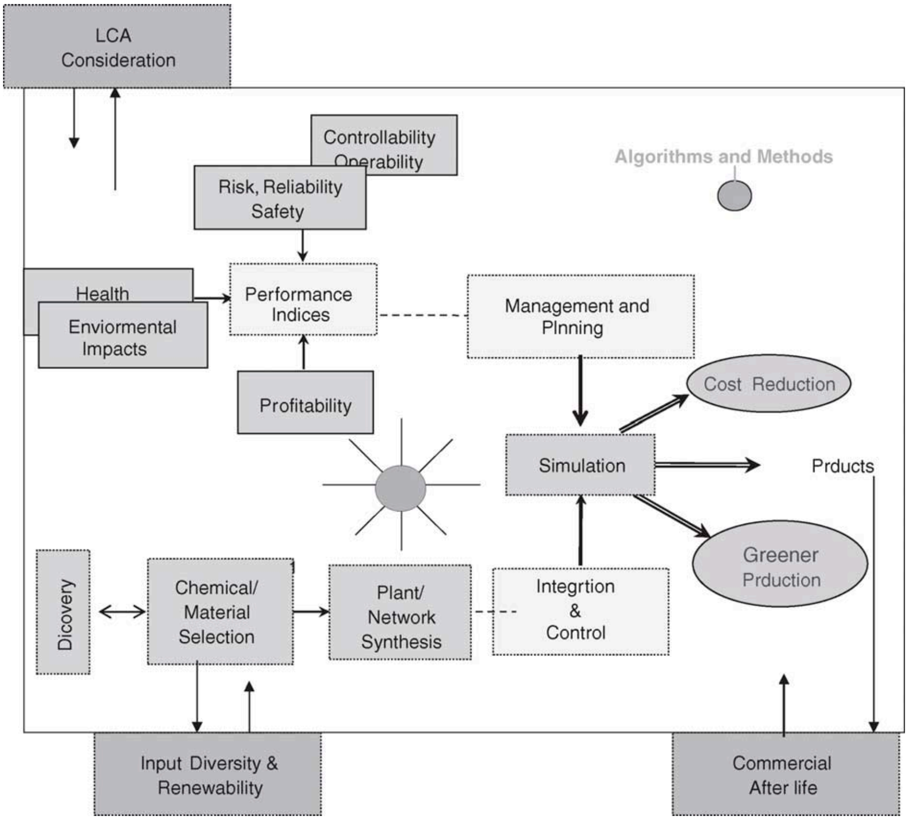

Fig. 1. Integrated framework for green engineering.

environmental impacts and superior performance. The details of the study can be found in a recent work (Subramanyan et al., ~~in press~~).

This involved solving a multi-objective optimization problem. The mathematical representation for the problem is presented below.

$$
\begin{aligned}
&\min\ Z_1 = [\text{cost}] \\
&\max\ Z_2 = [\text{efficiency}] \\
&\min\ Z_3 = [\text{CO}_2] \\
&\max\ Z_4 = [\text{SOFC current density}] \\
&\max\ Z_5 = [\text{PEM current density}]
\end{aligned} \tag{1}
$$

$$
\begin{aligned}
\text{s.t.}\quad &\text{Power rating constraints} \\
&\text{Material and energy balances} \\
&\text{Design specifications}
\end{aligned}
$$

As is well known, mathematics cannot isolate a unique optimum when there are multiple competing objectives. Mathematics can at most aid designers to eliminate design alternatives dominated by others, leaving a number of alternatives in what is called the Pareto set (Hwang et al., 1980). Fig. 2a shows the Pareto optimal solutions for minimization of cost and CO_2 emissions, and efficiency maximization. It is clearly seen that the non-convex nature of the multi-objective optimization problem here results in regions of trade-offs, as well as regions of opportunities. For instance, the region around 0.35 kg/kWh CO_2 emissions and 57% efficiency indicates costs around \$1500–\$1600 per kW. Immediately adjacent to the upper left of this region one can select plant designs with approximately 10% lower emissions, 15% higher efficiency, and 30% lower costs. Furthermore, this approach helps identify the best technology, which will provide the smallest trade-offs between objectives. One such significant result is, for instance, the trade-offs between efficiency and cost in case of strict environmental regulations. Here, the decision maker can determine which alternative is the most suitable given current regulations and policies. Further, extending this study to cover a multitude of technologies and potential resources will allow the determination of the most promising renewable technologies for electricity generation. The results show that cost does not necessarily conflict with the environmental impacts all the time, and one can find optimal designs which will be both environmentally friendly and economically beneficial. However, these trade-offs are obtained using system level models developed in ASPEN Plus simulator. The question is, will these trade-offs change if models do not capture the complete physical phenomena?

As stated earlier this technology is new and is at conceptual stage, therefore, we are considering the first type of uncertainties, i.e. uncertainties related to the modeling phenomena. Specially, we are concentrating on the two fuel cell models in this study. In general, an essential component (apart from the electrochemical reactions) of a fuel cell model is the current density characteristic of a particular fuel cell. The current density characteristic provides the voltage and current density profile, and is a function of fuel cell design. In this work, we have used the experimental data reported in the literature (Geisbrecht, 2002) to characterize uncertainties in the current density characteristic. Once probability distributions are assigned to the uncertain parameters, the next step is to propagate the uncertainties and obtain stochastic multi-objective optimization trade-off surfaces. Fig. 2b shows such a surface for the same three objective functions shown earlier in Fig. 2a. It can be seen that the modeling uncertainties have considerable effect on the objectives since the trade-off surfaces are markedly different. These uncertainties can be reduced if better models are used. However, obtaining the Pareto set for a highly nonlinear system like the hybrid fuel cell power plant is computationally very expensive even with simplified models used in this exercise. Inclusion of uncertainties results in many fold increased computational intensity. Therefore, it is necessary to have efficient methods, algorithms, and better computational power to address these problems. One such framework is described below.

2.2. Algorithmic framework

The algorithmic framework behind the integrated framework in Fig. 1, is shown in the Fig. 3.

Level 1, is the inner most level and corresponds to models for process simulation. This level defines all possible chemical and process alternatives for a particular process. Chem-

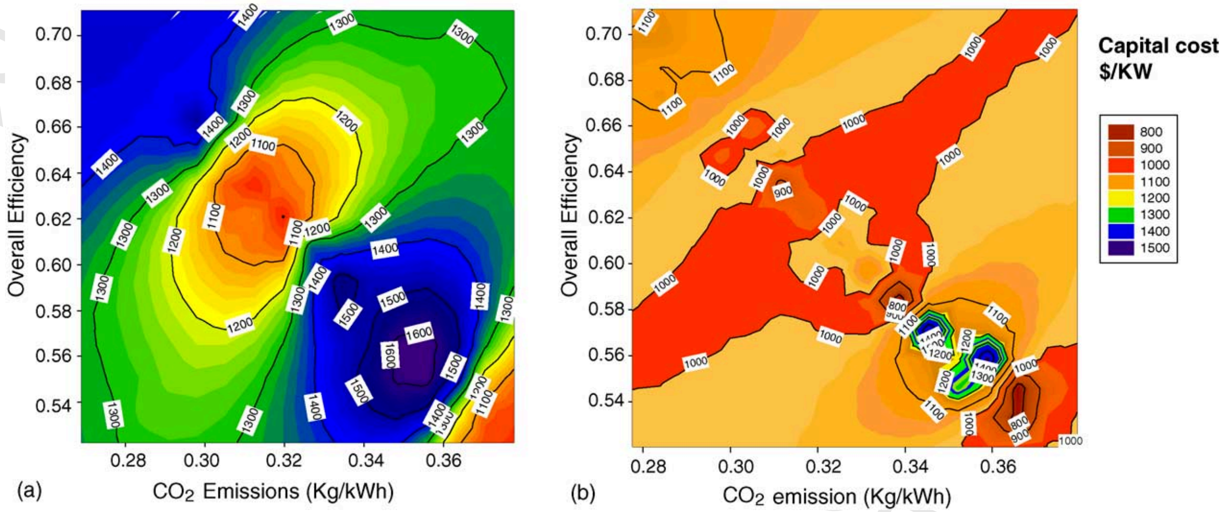

Fig. 2. Pareto-optimal surface for SOFC-PEM hybrid fuel cell power plant: (a) deterministic, (b) stochastic.

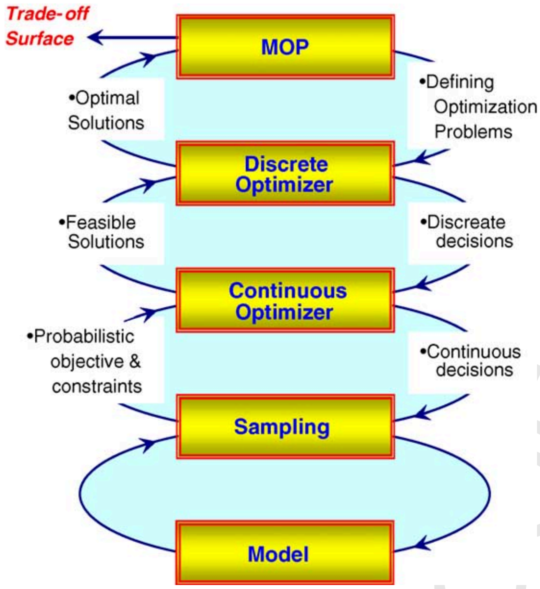

Fig. 3. The algorithmic framework.

ical process simulators like ASPEN (Aspen tech, 2003a), MultiBatchDS (Diwekar, 1996), SuperPro (Shanklin et al., 2001) are useful for this innermost level modeling.

Level 2, sampling loop: the diverse nature of uncertainty, such as estimation errors and process variations, can be specified in terms of probability distributions. The type of distribution chosen for an uncertain variable reflects the amount of information that is available. Once probability distributions are assigned to the uncertain parameters, the next step is to perform a sampling operation from the multi- variable uncertain parameter domain. Recently developed Hammersley sequence sampling (HSS) provides an efficient method for handling uncertainties in real world problems (Kalagnanam and Diwekar, 1997; Diwekar and Kalagnanam, 1997).

Level 3, continuous optimizer: this step involves continuous decisions like design and operating conditions for a process. Derivative based quasi-Newton methods, where the gradient (i.e., Jacobian) is approximated based on differences in the x and $f(x)$ obtained from previous iterations, are widely used in process optimization.

Level 4, discrete optimizer: this involves dealing with discrete decisions such as chemical and process structural alternatives. This is the most difficult optimization step. New algorithms are designed by improving efficiency in this discrete optimization step (Diwekar, 2003b; Kim and Diwekar, 2002).

Level 5, multi-objective programming, MOP: this represents the outermost loop in Fig. 3. A generalized multi-objective optimization problem can be formulated as follows:

$$\begin{aligned} \min \quad & Z = Z_i,\ i = 1, \ldots, p, \quad p \geq 2, \\ \text{s.t.} \quad & h(x, y) = 0, \\ & g(x, y) \leq 0, \end{aligned} \tag{2}$$

where x and y are continuous and discrete decision variables, and p is the number of objective functions like cost, and environmental impacts. The functions $h(x,y)$ and $g(x,y)$ represent equality and inequality constraints, respectively. There are a large array of analytical techniques to solve this MOP problem; however, the MOP methods are generally divided into two basic types: preference-based methods and generating methods. Preference-based methods like goal programming attempt to quantify the decision-maker's preference, and with this information, the solution that best satisfies the decision-makers's preference is then identified (Diwekar, 2003b). Generating methods, such as the weighting method and the constraint method, have been developed to find the exact Pareto set or an approximation of it. A new variant of constraint method that minimizes the number of single objective optimization problems (MINSOOP) to be solved can be used to obtain the Pareto set for green process designs (Fu and Diwekar, ~~in press~~).

As this framework is extended from process design to industrial ecology, data requirements increases and so are uncertainties. A conceptual approach based on various physical and thermodynamic constraints, optimization and uncertainty analysis algorithms and artificial intelligence method are presented below.

3. Industrial ecology and industrial symbiosis

Industrial ecology is the study of the flows of materials and energy in industrial and consumer activities, of the effects of these flows on the environment, and of the influences of economic, political, regulatory, and social factors on the use, transformation, and disposition of resources (White, 1994). Industrial ecology applies the principles of material and energy balance, traditionally used by scientists and engineers to analyze well-defined ecological systems or industrial unit operations, to more complex systems of natural and human interaction. These systems can involve activities and resource utilization over scales ranging from single industrial plants to entire sectors, regions or economies. In so doing, the laws of conservation must consider a wide range of interacting economic, social, and environmental indicators. Furthermore, new methods and data are required for identifying the appropriate principles and laws of thermodynamics for these higher levels of aggregation (Ayres, 1995a,b).

Fig. 4 presents a conceptual framework for industrial ecology applied at different scales of spatial and economic organization, evaluating alternative management options using different types of information, tools for analysis, and criteria for performance evaluation (Diwekar and Small, 2002). As one moves from the small scale of a single unit operation or industrial production plant to the larger scales of an integrated industrial park, community, firm or sector, the available management options expand from simple changes in process operation and inputs to more complex resource management strategies, including integrated waste recycling and reuse options. Special focus has been placed on implementing the latter via industrial symbiosis, for example, through the pioneering work of integrating several industrial and municipal facilities in Kalundborg, Denmark (Ehrenfeld and Gertler, 1997). At the higher levels of spatial and economic organization, at national and global scales, management is implemented through the tools of regulation, economic incentives, taxation, trade policy, and international agreements.

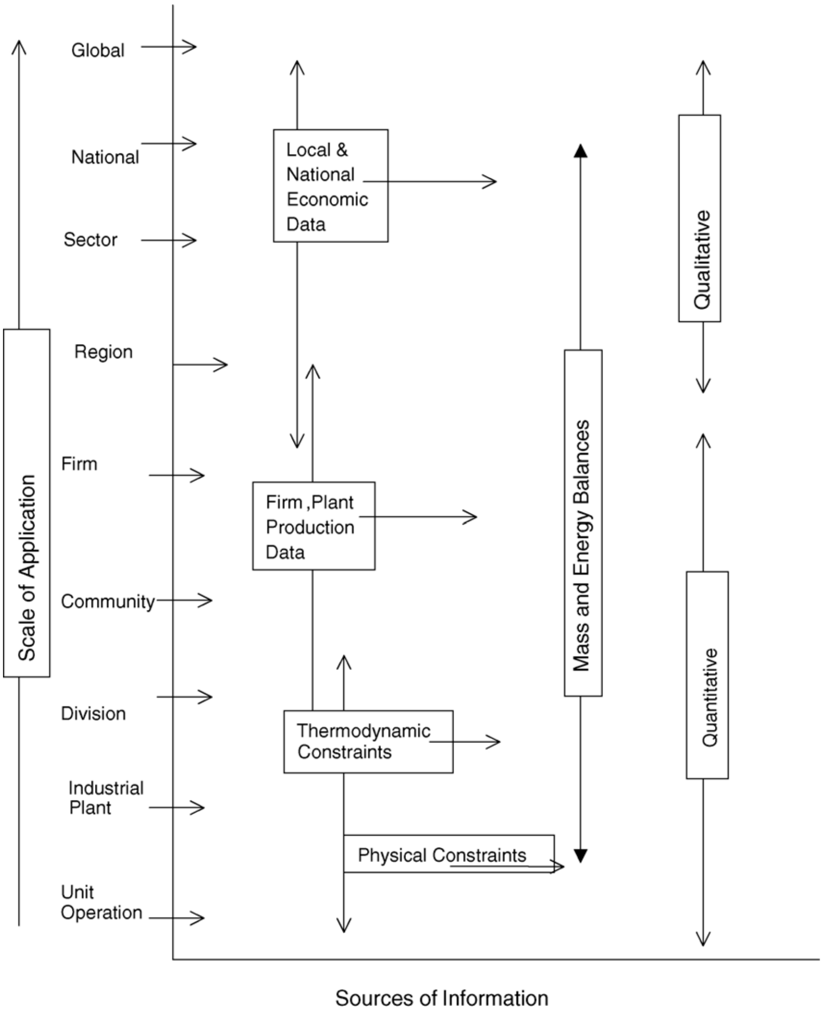

Fig. 4. Conceptual framework for industrial ecology.

To evaluate the full range of options illustrated in the framework shown in Fig. 4 apart from a multi-objective analysis (Chad and Allen, 1997), highly quantitative information on chemical properties, thermodynamic constants and constraints are needed, as are data relating to firm, sector, national and global resource utilization and conversion. Process simulators are based on mass and energy balance principles. They utilize thermodynamic models and data, and hence are ideally suited for imposing these constraints on the available data. However, the constraints and data involved are not restricted to mass and energy balance principles, and are available in various forms. For example, it is common practice to report undetectable quantities of emissions in terms of the detection limit (or least count) of the measuring instrument (specifying that the data may be less than or equal to the detection

Table 1
O(M) formalism and optimization constraints

O(M) relations	Verbal explanation	$r_L \leq r \leq r_U$		Constraints
		r_L	r_U	
r_1: $X_1 \ll X_2$	X_1 is much smaller than X_2	$-\infty$	e	$X_1/X_2 - r_1 = 0$
r_2: $X_1 -< X_2$	X_1 is moderately smaller than X_2	e	$1/1+e$	$X_1/X_2 - r_2 = 0$
r_3: $X_1 \sim< X_2$	X_1 is slightly smaller than X_2	$1/1+e$	1	$X_1/X_2 - r_3 = 0$
r_4: $X_1 = X_2$	X_1 is exactly equal to X_2	1	1	$X_1/X_2 - r_4 = 0$
r_5: $X_1 >\sim X_2$	X_1 is slightly larger than X_2	1	$1+e$	$X_1/X_2 - r_5 = 0$
r_6: $X_1 >- X_2$	X_1 is moderately larger than X_2	$1+e$	$1/e$	$X_1/X_2 - r_6 = 0$
r_7: $X_1 \gg X_2$	X_1 is much larger than X_2	$1/e$	∞	$X_1/X_2 - r_7 = 0$

e is the engineering tolerance.

limit). Sometimes, the data are reported in the order-of-magnitude terms (e.g., refer to Case 3 in (Ayres, 1995a), where the Benzo(a)pyrene content is reported to be much smaller than 0.0001). Furthermore, discrete, categorical information about the occurrence or non-occurrence of particular reactions, or the presence or absence of reaction byproducts, may be available.

Given that knowledge is available in various forms (e.g., quantitative models for material and energy balances, order-of-magnitude information, qualitative information, and logical information), a unified framework that incorporates information of each type into its inference is desirable. Optimization methods combined with artificial intelligence techniques, as proposed in (Kalagnanam and Diwekar, 1994), can provide such a framework. However, in order to describe this approach it is first necessary to choose a formal system which defines the syntax and the semantics for representing and reasoning with relative order of magnitude relations. The two main considerations for choosing a formalism is that it should provide an intuitive representation and should allow for sound and exact inferences. Here, we are using the O(M) formalism proposed by (Mavrovouniotis and Stephanopoulos, 1988). The optimization approach consists of first transforming the order of magnitude relations into a set of algebraic constraints (equality and inequality) as shown in Table 1 and then an optimization problem is solved for inference. Unlike numerical methods for solving equations (equality constraints), optimization methods can handle both equality and inequality conditions and hence can be used to make inferences from data in various forms.

4. Sustainability

One of the major problems in including industrial ecological concepts in design is the problem of uncertainties and defining broader metrics of overall resource use, global environmental and economical impacts. The topic of sutainability goes beyond industrial ecology and is, perhaps, operationally and conceptually one of the most complex that modern science has faced as it involves socio-economic interactions and its effect on the overall ecosystem. Fig. 5 presents the extension of framework from process design, to industrial ecology leading to socio-economic sustainability. At the center of this new framework is the green chemical plant engineered with clean products, clean processes, and green energy, and

Fig. 5. From green engineering to industrial ecology to sustainability.

eco-friendly management and planning as described in Fig. 1. The decision making is then extended to industrial symbiosis and industrial ecology, time-dependent socio-economic policies and together their effect on ecological systems leading to long term sustainability of the planet. However, it is necessary to provide a metric for sustainability that can address the cross disciplinary nature of sustainability involving human interactions with ecosystem. Fath and Cabezas (2002) have invoked the concept of information in its mathematical form as the centerpiece for their research work. The reason is that essentially any type of data or model can be converted to information regardless of disciplinary origin. Information can, therefore, serve as a common interdisciplinary bridge. They also hypothesized that information theory can serve as an appropriate basis for the construction of a basic theory of sustainability. The following brief paragraphs introduce Fisher information (FI) and their approach to a metric for sustainability.

The work of Fisher (1922) introduced a statistical measure of indeterminacy now called Fisher information. Fisher information can be interpreted as a measure of the ability to estimate a parameter, as the amount of information that can be extracted from a set of measurements, and also as a measure of the state of disorder of a system or phenomenon (Frieden, 1998). It is the later interpretation that has the most relevance to issues of sustainability. Fisher information, I, for one variable is calculated as follows:

$$\mathrm{FI} = \int \frac{1}{p(x)}\left(\frac{\mathrm{d}p(x)}{\mathrm{d}x}\right)^2 \mathrm{d}x \qquad (3)$$

which can be extended to a n-dimensional system. For physical systems, entropy follows the second law of thermodynamics, increasing monotonically with time. Conversely, Fisher information decreases with time as entropy (system disorder) increase. Ecological (and

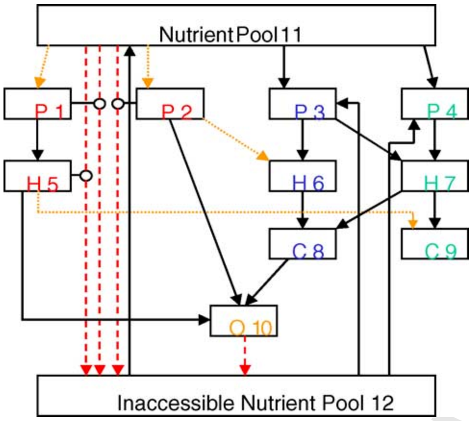

Fig. 6. Twelve compartment food web Model. Arrows indicate the direction of biomass.

perhaps sociological) systems, however, are able to create local order by utilizing energy flows through their self-organizing properties. This leads to the sustainability hypothesis proposed by Fath and Cabezas (2002).

The sustainability hypothesis states that: the time-averaged Fisher information of a system in a persistent regime does not change with time. The idea is that a change in regime will be manifest as a change in Fisher information. Note, this does not mean that changes that do not lead to a regime shift will not show up as changes in Fisher information.

However this hypothesis (this objective) involves dealing with various time scales and time dependent uncertainties which require appropriately modeling, and the solution methodology requires further development for arriving at decision domains.

4.1. A simple ecological model

Fig. 5 shows that in order to attain sustainability, one has to study the effect of various decisions from plant level to industrial sector to ecological level. Food web models is one way of studying the effect of waste on dynamics of the eco-systems. In order to study the sustainability hypothesis defined by the Fisher information, Cabezas and co-workers (Fath et al., 2003) used a simple food web model. In this work, the same model is used to show how human interventions like the change in mortality rates due to scientific advances, can perturb the dynamics of system. For more details, please refer to Duggempudi and Diwekar (2003).

The food web model consists of twelve compartments (Fig. 6):

1. Four primary producers i.e., plants (y_1–y_4).
2. Three herbivores (y_5–y_7).
3. Two carnivores (y_8, y_9).
4. An omnivore i.e., human (y_{10}).
5. Two nutrient compartments (y_{11} and y_{12}).

Compartment y_{11} is accessible to plants, which use the mass within it for their growth. Compartment y_{12} is inaccessible for consumption except to compartments y_3 and y_4, which bring this mass back into circulation. All compartments are limited in growth by resource availability. Mass balance on individual compartments results in the following equations:

$$\frac{\mathrm{d}y_i}{\mathrm{d}t} = y_i \left(\sum_{j=1}^{12} (g_i y_j - \epsilon_{ij} g_{ij} y_j) - \alpha_i \right) \quad i = 1, \ldots, 10 \tag{4}$$

where y_i is the biomass of the compartment, α_i is the mortality parameter, g_{ij} is the mass flow rate parameter between compartments i and j (i.e., consumption of mass from compartment i by species in compartment j), g_i is the growth rate of the compartment and ϵ_{ij} is a growth rate parameter such that $\epsilon_{ij} = 1$ if the mass flow rate is from compartment i to compartment j and $\epsilon_{ij} = -1$ if otherwise. The first two plants y_1 and y_2 are grown by humans. Hence, their growth depends upon the human population. This is incorporated by the following equations.

$$g_1 = g'_1 y_{10} \tag{5}$$

$$g_2 = g'_2 y_{10} \tag{6}$$

where g'_1 and g'_2 are the actual growth rates of the plants. The waste associated with cultivating these plants and the industrial waste in the model are represented as arrows passing through the circles projecting out of compartments 1, 2 and 5 in Fig. 6. The equations associated with these wastes are:

$$w_1 = w'_1 y_{10} \tag{7}$$

$$w_2 = w'_2 y_{10} \tag{8}$$

$$w_5 = w'_5 y_{10} \tag{9}$$

where w'_i is the "per capita" waste generation factor of compartment i. Also the consumption of plant y_2 by herbivore y_6 and of herbivore y_5 by carnivore y_9 is regulated by the humans by incorporating the following equations:

$$g_{26} = \frac{g'_{26}}{1 + y_{10}} \tag{10}$$

$$g_{59} = \frac{g'_{59}}{1 + y_{10}} \tag{11}$$

where g'_{26} and g'_{59} are the actual consumption rates. The arrows in Fig. 6 from the compartment 12 to plants y_3 and y_4 show the recycle rates (r_3 and r_4) from the inaccessible nutrient pool to these compartments. These recycle rates are input manually into the model. Compartment 11 is a passive sink for nutrient storage in which losses due to death accumulate.

Plants utilize this mass for growth, giving:

$$\frac{\mathrm{d}y_{11}}{\mathrm{d}t} = \sum_{j=1}^{12}(\alpha_j y_j) - y_{11}\left(\sum_{j=1}^{j=4} g_j y_j - \sum_{i=1,2,5} w_i\right) \tag{12}$$

where w_i is the waste factor of the compartment *i*. Compartment 12 is an inaccessible nutrient pool that acts as a sink for waste generated by humans (y_{10}) and the waste is involved in cultivation. Mass in y_{12} is re-introduced into the system by plants y_4 and y_3 in proportion to the mass in these compartments, with a low flow back to y_{11} representing long term recycling process:

$$\frac{\mathrm{d}y_{12}}{\mathrm{d}t} = \left(g_{12}y_{10} + y_{11}\left(\sum_{i=1,2,5} w_i\right) y_{12}(r_4 y_4 + r_3 y_3 + \alpha_{12}\right) \tag{13}$$

It has been assumed that all the four primary producers i.e., plants, are subject to sinusoidal forcing function to represent seasonal variation in growth due to solar incidence. The forcing function used in the model is:

$$g_i = \widehat{g_i}\left[1 + \frac{1}{3}\sin\left(\frac{2\pi t}{500} - \frac{\pi}{2}\right)^2\right] \quad i = 1, 2, 3, 4. \tag{14}$$

Using the above differential equations and taking the time period of integration as $T = 0$–1000 the Fisher information of the model is calculated by:

$$\mathrm{FI} = \frac{1}{T}\int_0^T \left(\frac{a(t)^2}{v(t)^4}\right)\mathrm{d}t \tag{15}$$

where $v(t)$ and $a(t)$ are the speed and acceleration of the system, respectively. These values are obtained from the 12 system variables by:

$$v(t) = \sqrt{\sum_{i=1}^{i=12}\left(\frac{\mathrm{d}y_i}{\mathrm{d}t}\right)^2} \tag{16}$$

$$a(t) = \frac{1}{vt}\left[\sum_{i=1}^{i=12}\frac{\mathrm{d}y_i}{\mathrm{d}t}\frac{\mathrm{d}^2 y_i}{\mathrm{d}t^2}\right]. \tag{17}$$

The model presented above is a deterministic model. However, a number of parameters in this model are prone to uncertainties. For example, it is a well-known fact that human mortality rates have changed over time due to breakthroughs in medicines and other scientific activities. Is it possible to model this time dependent uncertainties?

4.2. Modeling time dependent uncertainties

It is a common practice to use probability distribution functions like normal, lognormal, uniform distributions, to model uncertainties as shown in the earlier algorithmic framework.

However, these distributions are used for scalar parameter uncertainties. Modeling dynamic or time-dependent uncertainties is a difficult task. Recently, Diwekar (2003b) presented basic concepts for modeling time dependent uncertainties. These concepts are derived from the financial and economics literature where time dependent uncertainties dominate. The following paragraphs present these concepts briefly. This is followed by a subsection that uses analogy between stock prices and human mortality rate to develop models for time-dependent uncertainties in the rate of human mortality (Duggempudi and Diwekar, 2003).

4.2.1. Stochastic processes

A stochastic process is a variable that evolves over time in an uncertain way. One of the simplest examples of a stochastic process is the random walk process. The Wiener process or also called a Brownian motion is a continuous limit of the random walk and is a continuous time stochastic process. A Wiener process can be used as a building block to model an extremely broad range of variables that vary continuously and stochastically through time. For example, consider the price of a technology stock. It fluctuates randomly, but over a long time period has had a positive expected rate of growth that compensates investors for risk in holding the stock. Can the stock price be represented as a Wiener process? A Wiener process has three important properties:

1. It satisfies the Markov property. The probability distribution for all future values of the process depends only on its current value. Stock prices can be modelled as Markov processes, on the grounds that public information is quickly incorporated in the current price of the stock and past pattern has no forecasting value.
2. It has independent increments. The probability distribution for the change in the process over any time interval is independent of any other time interval (non-overlapping).
3. Changes in the process over any finite interval of time are normally distributed, with a variance that increases linearly with the time interval.

4.2.2. Human mortality rate: an Ito process

What is common between the technology stock price example and the uncertainty in the mortality rate parameter in the above discussed ecological model?

1. Both have time dependent variations. The technology stock fluctuates around the mean randomly, but over a long haul has a positive expected rate of growth. Mortality rates (from 1959 to 1999) on the other hand do not seem to show any trend but seem to fluctuate around a geometric mean as seen from Fig. 7. These mortality rates of human beings in the United States was collected from the years 1959 to 1999 from [http://www.mortality.org].
2. Similar to the stock prices, mortality rate can be modelled as a Markov process as at any time period. The changes for both are non-overlapping.

Hence, let us now assume that the behavior of the mortality rates with respect to time can be represented as a geometric mean reversion process (special instance of an Ito process), that is,

$$d\alpha = \eta(\bar{\alpha} - \alpha)dt + \sigma\alpha dz \tag{18}$$

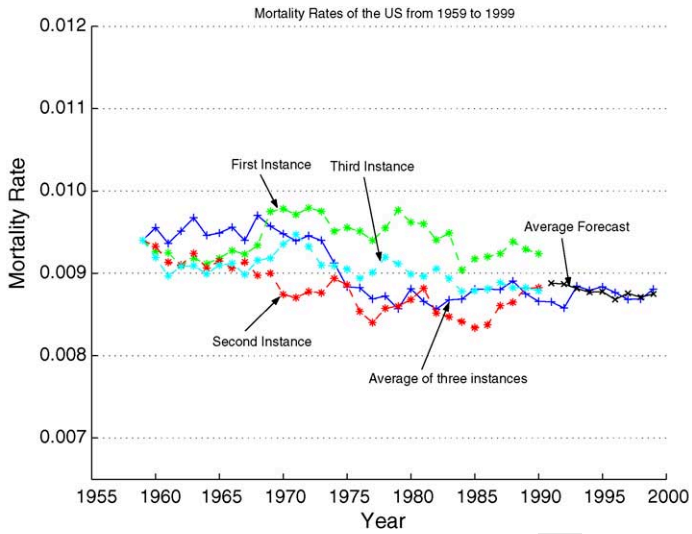

Fig. 7. Validation and forecasting of mortality rates as an Ito process.

In this process $\bar{\alpha}$ reverts to a mean α at a speed determined by the parameter η. The variance rate grows with α, so that the variance is zero if α is zero. In Eq. (18) dz is defined as $\mathrm{d}z = \epsilon_t \sqrt{\mathrm{d}t}$ where ϵ_t is drawn from a normal distribution with zero mean and unit standard deviation. A discrete time approximation to Eq. (18) is as follows:

$$\alpha_t - \alpha_{t-1} = \eta\bar{\alpha}\Delta t - \eta\Delta\alpha_{t-1} + \sigma\alpha_{t-1}\sqrt{\Delta t}\epsilon_t \tag{19}$$

where ϵ_t is $N(0, 1)$. Dividing through by α_{t-1} and using the notation:

$$c(1) = -\eta\Delta t \quad c(2) = \eta\bar{\alpha}\Delta t \quad e_t = \sigma\sqrt{\Delta t}\epsilon_t \tag{20}$$

The parameters of Eq. (20) can be estimated by running the regression on:

$$\frac{\alpha_t - \alpha_{t-1}}{\alpha_{t-1}} = c(1) + c(2)\frac{1}{\alpha_{t-1}} + e_t \tag{21}$$

The regression estimates are as follows: $c(1) = -0.07972$ and $c(2) = 0.0007049$. From the definitions of $c(1)$, $c(2)$ and e_t and given that Δt is taken as 1 year, the parameters are then estimated as $\eta = 0.079717$, $\sigma = 0.01538$ and $\bar{\alpha} = 0.008843158$.

Fig. 7 presents three sample paths from 1959 to 1990 of the above Ito process along with actual data. Each of the sample paths in Fig. 7 are an instance of the calculation of α based on Eq. (17). Also plotted is the average of these three paths from 1959 to 1990. Notice that ϵ_t is drawn from a normal distribution with zero mean and unit standard deviation, so, ϵ_t is a random number. The mortality rates are then forecast for the next 10 years from 1991 to 1999 to check if this process indeed captures the real data. As we can see from Fig. 7 the Ito process of Eq. (17) indeed captures the variability of the mortality rates from 1991 to 1999 and hence can be used to model the time dependent uncertainty and forecast their values in the future time.

4.3. Model revisited

The base case model for this problem presented earlier was deterministic in nature. The base case plot of Fisher information against the time over which it is integrated is shown in the Fig. 8. The Variance in the Fisher information, as can be seen from the Fig. 8, is found to be negligible showing a sustainable system. This is confirmed by the food web dynamics of the model with the masses of all the compartments as shown in the Fig. 9.

Now the time dependent uncertainties in the mortality rates were included in the model and the variance was calculated against the base case mean value of 0.1201. Fig. 10 shows the average Fisher information at each time step against the time. The variance in the Fisher information is computed to be 1.301810^6. This value is very high compared to the base case value, which shows that the uncertainties in the model parameters indeed increase the variance of the Fisher information. The food web dynamics of the model with uncertainties is shown in the Fig. 11. Notice from the dynamics of the model that even though we expect the human population to increase over time, the humans are indeed decreasing. This is because the food (or biomass) available for the humans for consumption is decreasing over time which decreases their population. Also seen is the tremendous increase in the population of the carnivore y_9. This decrease in the human population and increase in carnivore population is not favorable for the system. The system hence becomes unsustainable, and so the variance in the Fisher information increases. This suggest change in decision making or regulating some of the decisions. Optimization and optimal control methods can help in finding optimal regulations so as to offset these disturbances using stochastic dynamic programming. One can derive further from the real

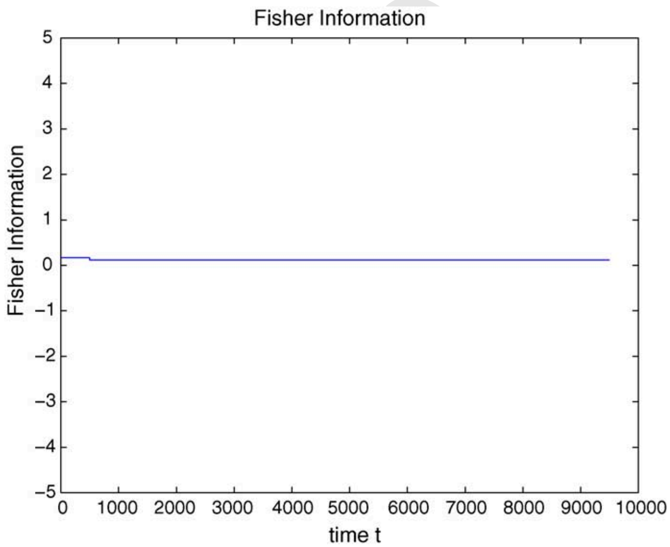

Fig. 8. Base case Fisher information plot.

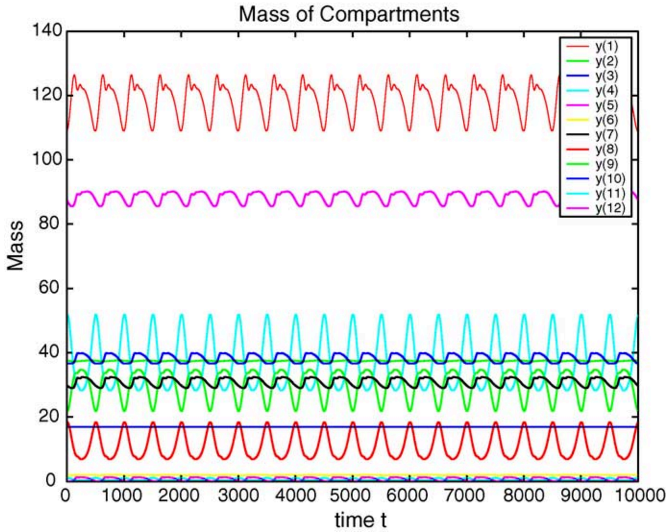

Fig. 9. Food web dynamics of the model at the base case.

options theory from finance. Most investment decisions share, to varying degrees, three important characteristics. First, the investment is partially or completely "irreversible". In other words, the initial cost of investment is at least partially "sunk"; you cannot recover it all should you change your mind. Second, there is "uncertainty" over the future rewards from the investment. The best you can do is to assess the probabilities of the alternative

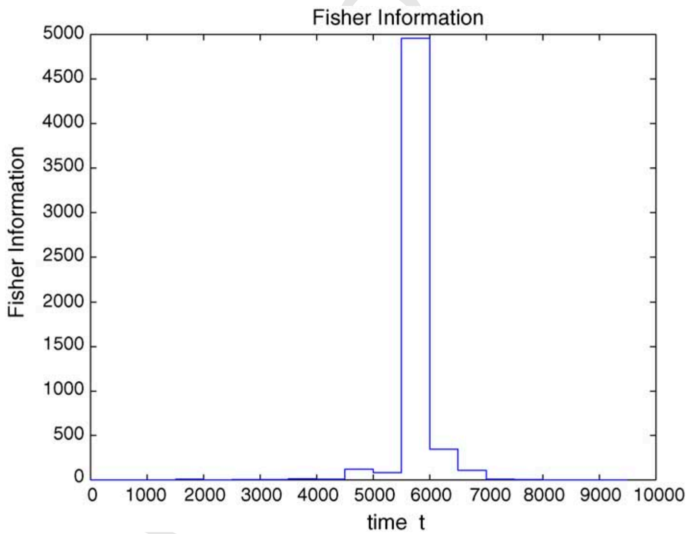

Fig. 10. Average Fisher information (at each time step when the uncertainties in the mortality rates are included).

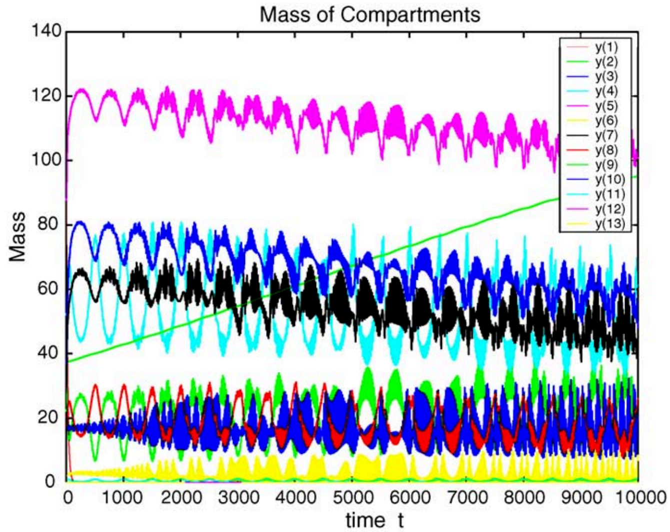

Fig. 11. Food web dynamics of the model (at the base case with uncertainties in the human mortality rates).

outcomes that can mean greater or smaller profit (or loss) for your venture. Third, you have some leeway on the "timing" of your investment. You can postpone action to get more information but not with complete certainty. These three characteristics interact to determine the optimal decisions or "options" for investors. A firm with an opportunity is holding an "option" to buy an asset at some future time of its choosing. When a firm makes an irreversible expenditure, it exercises, or "kills", its option to invest. This lost option value is an opportunity cost that must be included as part of the cost of investment. Also, this opportunity cost is highly sensitive to the uncertainty over the future value of the project. Options theory (Dixit and Pindyck, 1994) has been developed to make decisions in such an investment environment. Like investment decisions, decisions concerning the sustainability also involve elements of irreversibility, uncertainty, and the possibility of delay.

5. Summary

This paper presented the systems analysis approach that extends from process design to industrial ecology to overall sustainability. Green engineering concepts extended the traditional design framework by starting the decision making as early as the chemical and material selection stage and ending it with management and planning decisions. In order to take care of the uncertainties and various forms of decisions encountered in a nonlinear system of process design, an efficient algorithmic framework for multi-objective optimization under uncertainty is developed. However, uncertainties increase in design for environment, especially, when one has to deal with new greener technologies. A fuel cell based hybrid power plant designed using green engineering principles highlighted this aspect. Industrial ecology is the next step to process design where this decision making changes from the small scale of a single unit operation or industrial production plant to the larger scales of an integrated industrial park, community, firm or sector, and the available management options expand from simple changes in process operation and inputs to more complex resource management strategies, including integrated waste recycling and reuse options. Uncertainties increase in industrial ecology due to data unavailability and various level of model aggregation. Here, methods for handling various forms of knowledge are useful. The concept of overall sustainability goes beyond industrial ecology and brings in time dependent nature of the ecosystem. Time dependent uncertainties and short to long term decisions in the face of uncertainties makes decision making complicated. Further, with this interdisciplinary aspect of system requires a different matric for evaluating sustainability. Recently developed sustainability theory based on Fisher information can provide a viable multi-disciplinary metric. Time dependent uncertainties and forecasting the decision is a common practice in finance. Therefore, theories from finance literature along with optimal control and optimization algorithms can help in addressing this problem. A simple ecological case study illustrated this concept.

References

Aspen tech, 2003a. AspenTech. Aspen Plus 12.1 User Guide. Cambridge, MA: AspenTech; 2003.

Aspen tech, 2003b. AspenTech. Batch Plus 12.1 User Guide. Cambridge, MA: AspenTech; 2003.

Ayres R. Life cycle analysis: a critique. Resource Conserv Recycl 1995a;14:199.

Ayres R. Thermodynamics and process analysis for future economic scenarios. J Environ Resource Econ 1995b;6:207.

Anastas PT, Zimmerman JB. Design through the 12 principles of green engineering. Environ Sci Technol 2003;37(5):95–101.

Chad D, Allen D. Minimizing chlorine use: assessing the trade-o.s. between cost and chlorine use in chemical manufacturing. J Ind Ecol 1997;1(2):111–34.

Diwekar U. Understanding batch distillation process principles with multibatchds. Comput Appl Chem Eng Educ 1996;4(4):275–84.

Diwekar U. Greener by design. Environ Sci Technol 2003a;37:5432–44 [Invited paperdkjdot].

Diwekar U. Introduction to Applied Optimization. Dordrecht: Kluwer Academic Publishers; 2003b.

Diwekar U, Kalagnanam JR. Efficiency sampling technique for optimization under uncertainty. AIChE J 1997;43(2):440–7.

Diwekar U, Small M. Process analysis approach to industrial ecology. In: Ayres, Ayres, editors. A handbook of industrial ecology. UK: Edward Elgar; 2002. p. 115–37.

Dixit A, Pindyck R. Investment under uncertainty. Princeton, NJ: Princeton University Press; 1994.

J. Duggempudi, U. Diwekar 2003. Sustainability, options theory, and off-line quality control. In Sustainability and Life Cycle Topical Conference, San Francisco, CA: AIChE National Meeting; 2003. p. 155C.

Ehrenfeld J, Gertler. Industrial ecology in practice: the evolution of interdependence at kalundborg. J Ind Ecol 1997;1(1):67.

EPA. WAste Reduction (WAR) Algorithm Graphical User Interface, Version 1.0. ORD, US EPA; November, 2002.

Fath B, Cabezas H. Towards a theory of sustainable systems. Fluid Phase Equil 2002;2:194–7.

Fath B, Cabezas H, Pawlowski C. Regime changes in ecological systems: an information theory approach. J Theor Biol 2003;222(4):517–30.

R. Fisher. Phil Trans Royal Soc Lond 1922;222:309.

Frieden B. Physics from Fisher information: a unification. Cambridge, United Kingdom: Cambridge University Press; 1998.

Y. Fu, U. Diwekar. An efficient sampling approach to multi-objective optimisation, Ann Operat Res, ~~in press,~~

R. Geisbrecht, 2002. Theory based process modeling for evaluation of fuel cells in advanced energy systems. Topical conference on Fuel Cells Power Systems. New Orleans, LA: AIChE Spring National Meeting, 2002.

Ei-Halwagi MM. Pollution prevention through process integration: systematic design tools. San Diego, CA: Academic Press; 1997.

Hwang CL, Paidy SR, Masud ASM. Mathematical programming with multiple objectives: a tutorial. Comput Operat Res 1980;7:5–31.

Kalagnanam J, Diwekar U. An optimization approach to order of magnitude reasoning. AI Eng Des 1994;8:207.

Kalagnanam JR, Diwekar U. An efficient sampling technique for off-line quality control. Technometrics 1997;39(3):308–19.

Kim K-J, Diwekar U. Hammersley stochastic annealing: Efficiency improvement for combinatorial optimization under uncertainty. IIE Trans Operat Eng 2002;34(9):761–78.

Mavrovouniotis M, Stephanopoulos G. Formal order-of-magnitude reasoning in process engineering. Comput Chem Eng 1988;12:867–80.

Molecular Knowlege Systems. Synapse Designer's Guide. Cambridge, MA: Molecular Knowledge Systems, Inc., 1994.

Molecular Knowlege Systems. Cranium User's Guide. Cambridge, MA: Molecular Knowledge Systems, Inc., 1998.

Rossiter A. Process integration and pollution prevention. In: Ei-Halwagi M, Petrides D, editors. Pollution prevention via process and product modifications. New York, NY: American Institute of Chemical Engineers; 1994.

Shanklin T, Roper K, Yegneswaran PK, Marten M. Selection of bioprocess simulation software for industrial applications. Biotechnol Bioeng 2001;72(4):483–9.

K. Subramanyan, U. Diwekar, A. Goyal. Multi-objective optimization for hybrid fuel cells power system under uncertainty. J Power Sources, ~~in press,~~

White A. Preface. In: The greening of industrial ecosystems. Washington, DC: National Academy of Engineers, National Academy Press; 1994.