Green process design, green energy, and sustainability: A systems analysis perspective

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Abstract

This paper presents a systems analysis perspective that extends the traditional process design framework to green process design, green energy and industrial ecology leading to sustainability. For green process design this involves starting the design decisions as early as chemical and material selection stages on one end, and managing and planning decisions at the other end. However, uncertainties and multiple conflicting objectives are inherent in such a design process. Uncertainties increase further in industrial ecology. 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. Decision making at various stages starting from green process design, green energy, to industrial ecology, and sustainability is illustrated for the mercury cycling. Power plant sector is a major source of mercury pollution. In order to circumvent the persistent, bioaccumulative effect of mercury, one has to take decisions at various levels of the cycle starting with greener power systems, industrial symbiosis through trading, and controlling the toxic methyl mercury formation in water bodies and accumulation in aquatic biota.

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1. Introduction

Chemical process simulation tools and models allow engineers to design, simulate and optimize a process. Steady state simulators like PRO-II and ASPEN Plus are well known in this area and are extensively used for the simulation of continuous processes. In recent years, chemical process industries have become aware of the importance of waste reduction, and environmental consciousness demands an effort extending far beyond the capability of existing process simulation to model processes with environmental control options. For tracking trace components nonequilibrium-based models are implemented. Packages like Waste Reduction Algorithm (WAR) (EPA, 2002) provide data related to various environmental impacts like toxicity and exposure data. Designing green processes with “process integration” which takes into consideration the entire process is now possible with the new tools. However, there is still a long way to attain the goal of sustainability. Unlike traditional design where engineers are looking for low cost options, environmental considerations include objectives like the long-term and short-term environmental impacts. Green process design and green energy involve not only extending the design framework to include process integration, environmental control technologies, starting as early as the material selection stage, and going beyond just green energy, green processing, and green management, but also to look at industrial sector level management through industrial ecology as shown in Fig. 1. 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 integrated industrial park, community, firm or sector. Uncertainties increase as one goes from traditional process design to green design and to industrial ecology. The concept of overall sustainability goes beyond industrial ecology and brings in time dependent nature of ecosystem. Decisions regarding regulations, human interactions with ecosystem come in picture. It involves dealing with various time scales and time dependent uncertainties. This work presents a systems analysis approach to various steps involved from green process design to sustainability.

Mercury has been recognized as a global threat to our ecosystem, and is fast becoming a major concern to the environmentalist and policy makers. Mercury is a major pollutant from power plants. The task of mercury pollution management is arduous due to the complex environmental cycling of mercury compounds. Successful handling of the issues calls for a sustainability-based approach. This work presents the systems analysis approach to sustainability with the case study of mercury. The next section briefly describes the mercury cycle that highlights its complex nature. This discus-
2. Mercury cycle

Mercury can cycle in the environment in all media as part of both natural and anthropogenic activities (USEPA, 2000a,b). Majority of mercury is emitted in air in elemental or inorganic form, mainly by coal fired power plants, waste incinerators, industrial and domestic utility boilers, and chloro-alkali plants. However, most of the mercury in air is deposited into various water bodies such as lakes, rivers and oceans through processes of dry and wet deposition. In addition, the water bodies are enriched in mercury due to direct industrial wastewater discharge, storm water runoffs, and agricultural runoffs. Once present in water, mercury is highly dangerous not only to the aquatic communities but also to humans through direct and indirect effects. Methylation of inorganic mercury leads to the formation of methyl mercury which accumulates up the aquatic food chains, so that organisms in higher trophic levels have higher mercury concentrations (DeSimone et al., 1973; Jensen & Jernelov, 1969). The consumption of these aquatic animals by humans and wild animals further aids the bioaccumulation along the food chain. As a result, contaminated fish consumption is the most predominant path of human exposure to mercury. This has resulted in fish consumption advisories at various water bodies throughout the US. Given this complex cycling, management options at multiple stages must be considered to effectively mitigate the impact. The work proposes sustainable management strategies at various levels of mercury cycle:

- Industry level environmental control technologies selection and design.
- Industrial sector (inter-industry) level symbiosis through trading, combined with industry level management resulting in Mixed Integer Nonlinear Programming (MINLP) and Stochastic Mixed Integer Nonlinear Programming (SMINLP) problems.
- Ecosystem level management: effective control strategies of mercury bioaccumulation in water bodies. These strategies are given below.
  - Lake pH control to manage methyl mercury formation.
  - Manipulation of the regimes of species population by controlling Fisher information variation.

Optimal control and stochastic optimal control methods are used for these strategies.

In order to succeed in these objectives, various techniques and systems theory tools need to be used and integrated. The following section presents these tools and the algorithmic framework for this work.

3. Algorithmic framework

The algorithmic framework is shown in Fig. 2. The optimization framework is used for green process design and industrial ecology, while stochastic optimal control is used for time dependent decisions under uncertainty.

Level 1: It is the inner most level and corresponds to models for processes. For ecological level management, at this level optimal control and stochastic optimal control problems are formulated. Optimal control problems in engineering have received considerable attention in the literature. In general, solutions to these problems involve finding the time dependent profiles of the decision (control) variables so as to optimize a particular performance index. The dynamic nature of the decision variables makes these problems much more difficult to solve compared to normal optimization where the decision variables are scalar. In general, mathematical methods to solve these problems involve calculus of variations, the maximum principle and the dynamic programming technique. Nonlinear Programming (NLP) techniques can also be used to solve this problem provided all the system of differential equations is converted to nonlinear algebraic equations. For details of these methods, please see Diwekar (2008). In the maximum principle, the objective function is reformulated as a linear
function in terms of final values of state variables and the values of a vector of constants resulting in ordinary differential algebraic equation that are easier to solve as compared to calculus of variations or dynamic programming. However, this maximum principle formulation needs to include additional variables and additional equations. We use the maximum principle and the stochastic formulation to model 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.

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. 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.
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.

Stochastic processes like Weiner processes do not have time derivatives in the conventional sense and, as a result, they cannot be manipulated using the ordinary rules of calculus as needed to solve the stochastic optimal control problems. Ito provided a way around this by defining a particular kind of uncertainty representation-based on the Wiener process. An Ito process is a stochastic process $x(t)$ on which its increment $dx$ is represented by the equation:

$$dx = a(x, t) dt + b(x, t) dz$$

where $dz$ is the increment of a Wiener process $(dz = \epsilon \sqrt{dt})$, and $a(x, t)$ and $b(x, t)$ are known functions. $\epsilon$ is a unit normal distribution. 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. Hammersley sequence sampling (HSS) provides an efficient method for handling uncertainties in real world (Diwekar, 2008; Kalagnanam & Diwekar, 1997) and is used here.

**Level 3:** Continuous optimizer: This step involves continuous decisions like design and operating conditions for a process. Derivative-based quasi–Newton methods are used for this step.

**Level 4:** Discrete optimizer: This involves dealing with discrete decisions such as various point sources and environmental control options. Decomposition strategies are used for MINLP problems.

**Level 5:** Multi-Objective Programming (MOP): This represents the outermost loop in Fig. 2. There is 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-maker’s preference is then identified. 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 (MNSOOP) (Fu & Diwekar, 2004) to be solved which is based on the HSS method can be used for this framework. HSS method can be combined with the weighting method also.

The rest of the article elaborates on this integrated systems analysis approach by presenting a case study of mercury pollution management where this approach can be extremely valuable. However, before these specific approaches are discussed, the next section briefly describes the case study.

### 4. Savannah River watershed case study

Total Maximum Daily Load (TMDL) of 32.8 kg/year, which represents the maximum permitted cumulative loading for the watershed, has been established by the USEPA for five contiguous segments of the Savannah River in the state of Georgia, US, leading to the applicable water quality standard (WQS) of 2.8 ng/l (parts per trillion) in the watershed (USEPA, 2001). In all, there are 29 significant point sources (PS) discharging mercury in the watershed, including 13 major municipal polluters, 12 major industrial polluters, 2 minor municipal polluters and 2 minor industrial polluters. The TMDL is implemented by applying the common WQS of 2.8 ng/l to all PS discharges across the watershed. The sum of the individual waste load allocations is 0.001 kg/year, which is significantly less than 0.33 kg/year, the cumulative waste load allocation provided to all PS (USEPA, 2001). This difference appears because there are 50 more point sources in the watershed that were ignored, either because the discharges were very small or not measurable with certainty. The overall reduction needed to achieve the TMDL is about 44% (USEPA, 2001). Since the current discharge concentrations for the 29 point sources are not reported in the literature, the individual discharge values are computed by taking 29 random samples so that the mean required reduction for the watershed based on the WQS is about 44%.

### 5. Industrial level and industrial sector level mercury management

In the wake of increasingly stringent discharge regulations on mercury, efficient management at the individual level is not suf-
efficient. Innovative methods are required that will analyze the problem from industrial sector level achieving simultaneous economic and ecological sustainability.

5.1. Industrial level management: environmental control technologies

Three environmental control technologies are considered for this problem and they are available to all industries for implementation. These include: coagulation and filtration, activated carbon adsorption and ion exchange process. The capital requirement and reduction capability of any process is expected to be nonlinearly related to the capacity of the treatment plant and the form and concentration of the waste to be treated, amongst many other factors. The total plant cost is reported as a function of the waste volume (USDOI, 2001). Since waste volumes encountered in this case study are mostly greater than 1 MGD, asymptotic values reported in USDOI (2001) are used. The treatment efficiencies depend on the waste composition and concentration. In general though, a more efficient treatment is likely to be more expensive. This criterion, along with data given in USEPA (1997a), is used to decide the treatment efficiencies. Table 1 gives the technology data. The nonlinear cost functions are reported in USEPA (1997b). The models are not reproduced here for the sake of brevity and interested readers are referred to the mentioned reference.

5.2. Industrial sector level management: pollutant trading

Pollutant trading is a market-based strategy to economically achieve environmental resource management. The goal is to attain the same or better environmental performance with respect to pollution management at a lower overall cost for the industrial sector. The concept is attributed to Crocker (1966), Dales (1968), and Montgomery (1972).

Various aspects of watershed-based trading are extensively discussed in USEPA (1996, 2003) and hence not reproduced here. To summarize the aspects relevant for this work, the state or federal authority proposes a regulation such as Total Maximum Daily Load (TMDL) which establishes the loading capacity of a defined watershed, identifies reductions or other remedial activities needed to achieve water quality standards, identifies sources, and recommends waste load allocation for point (and nonpoint) sources. To comply with the regulation, a point source (industry) in the watershed may need to reduce its discharge level. It has two options to accomplish this: (1) the point source can implement an environmental control technology; (2) the point source can trade a particular amount of pollutant to another point source in the watershed that is able to reduce its discharge more than that specified by the regulation.

5.2.1. Trading optimization problem formulation

The formulation considers that a TMDL (Total Maximum Daily Load) regulation has already been developed by the state in consultation with USEPA. This translates into a specific load allocation for each point source. Consider a set of point sources \( PS_i \), \( i = 1, \ldots, N \), disposing mercury containing wastewater to a common water body or a watershed. Let \( j = 1, \ldots, M \) be the set of waste reduction technologies available to the point sources. Let \( D_i \) be the discharge quantity of polluted water from \( PS_i \) [volume/year], \( r_d \) be the desired pollutant quantity reduction in discharge of \( PS_i \) [mass/year], \( P_i \) be the treatment cost incurred by \( PS_i \), in absence of trading, and \( f_j(\phi_j, D_i) \) be the linear or nonlinear cost function for technology \( j \) at \( PS_i \) [\$/]. Here, \( \phi_j \) is the set of design variables for technology \( j \). \( q_j \) is the pollutant reduction possible from technology \( j \) implementation [mass/volume]. \( r \) is the trading ratio, defined as the number of units of reduction that must be purchased to trade one unit of the pollutant and which is typically higher than 1 to account for reduction uncertainties, and \( F \) is the transaction cost, which is the amount paid by the point source for trading one unit of pollutant [\$/mass]. The trading optimization problem is then formulated as:

\[
\text{Minimize } \sum_{i=1}^{N} \sum_{j=1}^{M} f_j(\phi_j, D_i) \cdot b_{ij} \quad (2)
\]

\[
t_{ii} = 0 \quad \forall i = 1, \ldots, N \quad (3)
\]

\[
\text{red}_d \leq \sum_{j=1}^{M} q_j \cdot D_i \cdot b_{ij} + \sum_{k=1}^{N} t_{ki} - r \sum_{k=1}^{N} t_{ki} \quad (4)
\]

\[
P_i = \sum_{j=1}^{M} b_{ij} \cdot f_j(\phi_j, D_i) + F \left( \sum_{k=1}^{N} t_{ki} - \sum_{k=1}^{N} t_{ki} \right) \quad (5)
\]

where \( b_{ij} \) are the binary variables representing point source technology correlation. The variable is 1 when a point source installs technology \( j \). \( t_{ii} \) [mass/year] is the amount of pollutant traded by \( PS_i \) with \( PS_i \). All parameters are on an annual basis. The objective function gives the sum of the technology implementation costs for all point sources. Although each PS will also spend or gain from practising trading, expense for one PS in a watershed is earning for one or more PS in the same watershed. As a result, for the complete watershed, trading does not contribute to the cost objective. The first set of constraints eliminates trading within the same PS. The second set of constraints ensures that all the regulations are satisfied, with or without trading. The trading ratio \( r \) is usually set higher than 1 to account for data uncertainty and provide a buffer (USEPA, 1996). Consequently, the PS accepting additional discharge reduction responsibility has to reduce the pollutant by an amount equal to the actual quantity traded \( t_{ii} \) times the trading ratio. The last constraint ensures that the expenses incurred by each PS with trading are not more than those without trading. Since participation in trading is voluntary, a polluter will participate in trading only if there is a financial incentive, which is modeled by this constraint. Moreover, since transaction costs are paid on the basis of the actual amount traded, the trading ratio is not included in the final constraint. It is considered that trading is possible between all point sources. For simplicity, a single trading policy exists between all possible pairs of point sources, and a single trading ratio \( r \) and transaction fee \( F \) is applicable to all the trades.

The proposed model is applied to the Savannah River watershed. There are 29 major polluters in this watershed including a power plant.

5.2.2. Uncertainty consideration

The optimization model presented above assumes that all data is deterministically known. However, there are various possible sources of uncertainty in this framework. For example, the Mercury Study Report to Congress (USEPA, 1997b) states that uncertainty in point estimates of anthropogenic mercury emissions ranges from medium (25%) to high (50%). A stochastic optimization (stochastic programming) problem must be formulated to account for these uncertainties. In this work, the deterministic formulation is:

<table>
<thead>
<tr>
<th>Process</th>
<th>Mercury reduction capability (ng/l)</th>
<th>Capital requirement ($/1000 gallons)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Activated carbon adsorption (A)</td>
<td>3.0</td>
<td>1.5</td>
</tr>
<tr>
<td>Coagulation and filtration (B)</td>
<td>2.0</td>
<td>1.0</td>
</tr>
<tr>
<td>Ion exchange (C)</td>
<td>1.0</td>
<td>0.6</td>
</tr>
</tbody>
</table>
extended to include uncertainty in the cost functions of the various control technologies. The resulting stochastic programming problem is computationally difficult to solve. Hence, the problem is converted into a two stage stochastic programming problem and established techniques from stochastic programming are used to solve the problem efficiently.

5.2.3. Health care cost
The bioaccumulative nature of mercury and its slow dynamics make the long-term effects of mercury exposure important. Hence, it is essential to account for such effects while quantifying health care costs. Majority of mercury accumulates in the food chain as methyl mercury. Therefore, quantification of health care costs based on methyl mercury concentration is most appropriate. Health care cost is assumed to be a function of fish consumption, safe concentration in fish, and LC50 value for mercury. Addition of health care cost in the formulation results in a multi-objective optimization problem, where compliance cost and health care cost are the two objectives.

5.2.4. Results and discussions
Fig. 3 plots the annual saving due to trading implementation for the considered TMDL range (26–36 kg/year) for three different models. It is observed that approximate linear models underestimate the annual savings. Inclusion of uncertainty in the analysis predicts even higher savings for most TMDL values. It should be noted here that trends in savings do not necessarily reflect the trends in overall cost. Thus, although nonlinear stochastic model leads to higher savings than nonlinear deterministic model, the total cost with trading for nonlinear stochastic model is not necessarily lower than the total cost with trading for nonlinear deterministic model. This is because the savings for a particular model are calculated over the technology option for the same model setting.

Fig. 4 shows the implications of nonlinearity and uncertainty inclusion on technology selection for trading option. The figure shows the number of times each technology is implemented over the complete TMDL range. It can be seen that there are definite implications on technology selection. With linear technology models, various small industries implement technologies along with large industries. However, for nonlinear model, large industries implement most of the technologies and smaller industries satisfy the regulations by trading with these large industries.

5.2.5. Multi-objective problem
The multi-objective optimization problem in the presence of uncertainty was solved using the weighting method. Here, each objective in the cumulative objective function is multiplied by a coefficient, which is called as the weight on that objective. Higher value of the weight for a particular objective represents greater importance of that objective in the cumulative objective function. In this analysis, the weight on the cost-based objective is maintained at 1 while the weight on the health care cost is progressively increased from 50 to 500, indicating greater importance to health care cost. Fig. 5 shows the cumulative distribution of technology selection by different point sources for various TMDL values for different weights. It illustrates a preference towards the selection of a more efficient treatment technology. It must be noted that the granular activated carbon adsorption was the most efficient and most expensive technology while ion exchange was the least efficient and least expensive technology. The percentage of activated carbon adsorption increased from 49.28% for the weight of 50, to 57.88% for the weight of 500. On the contrary, the percentage of coagulation and filtration decreased and that of ion exchange remained almost the same. Moreover, the total number of times technologies are implemented also increased from 69 for the weight of 50, to 311 for the weight of 500. It must be noted that these are cumulative values for different optimization problem solutions at 11 different TMDL values (26–36 kg/year). This result, combined with the increased percentage, pointed towards a significant preference for very efficient technology. This further highlights the point that increased importance of health care cost can change the optimal solution of a pollutant trading problem.

6. Ecological level management
Mercury and its compounds exist in different segments of the water body such as water column, sediment (active and passive), and biota (fish). Mercury can undergo various transformations in a
water body such as oxidation, reduction, volatilization, methylation and demethylation. All these transformations are simultaneously observed in a given water body. The relative concentration of each chemical form depends on the extent of various reactions, which can differ for different water bodies. Of the various chemical forms of mercury, methyl mercury (MeHg) is considered to be the most dangerous due to its bioaccumulative potential. As a result, the concentration of methyl mercury in large aquatic animals (such as predatory fishes) is many times more than the water column or sediment concentration. This work explores two strategies for ecosystem mercury management: (1) time dependent liming strategy of lakes and rivers to control water pH and (2) controlling nutrient flow to manipulate eating habits of organisms.

6.1. Liming and pH control

Methylation of mercury to MeHg is a key step in the bioaccumulation of mercury in aquatic food chains (Sorensen, Glass, Schmidt, Huber, & Rapp, 1990). The exact mechanism of the methylation reaction is however not well understood. Studies have also been carried out to understand the effect of physical and chemical conditions such as pH, dissolve oxygen, dissolved organic carbon (DOC), temperature, salinity, etc., on methylation (Driscoll et al., 1995; Winfrey & Rudd, 1990). These studies have shown a strong correlation between acidic conditions (low pH values) and high mercury bioaccumulation in fish. Therefore, lake liming, which means addition of lime to a given water body, has been proposed as a management tool. This controls the pH, therefore, should lead to less MeHg formation and consequently less bioaccumulation.

It is a valuable short-term management option that can be implemented on a case-by-case basis till the original problems of mercury pollution and acid runoffs are satisfactorily addressed.

Although lake liming for pH control has been relatively successful in Scandinavian countries, there are various issues related to liming that need further in-depth research. These are:

1. Liming accuracy: Currently, most of the liming decisions (liming dosage) are based on rule of thumb. The amount of lime to be added is decided using parameters such a lake volume, current lake pH, targeted pH, water salinity, etc. (Hakanson & Boulion, 2002). These are mostly static decisions and do not take into account the dynamic nature of the natural system. It is obvious that such heuristics-based decisions do not lead to accurate liming results.

2. Cost of liming: Liming entails considerable costs. Hence, it is essential that the liming operation is optimized to reduce expenses. Even though the liming technique is the major factor deciding the expenses, efficient implementation of the selected technique can reduce expenses. Previous work in this area includes Hakanson (2003) and Riely and Rockland (1988).

3. Presence of uncertainty: Liming operation has to deal with presence of various kinds of uncertainties, such as lack of information on the exact pH of the lake, seasonal variations in lake pH, and topological effects of liming. Moreover, the spatial and temporal effects of liming on lake biota are subjective. In order to make liming implementable, one needs to incorporate these uncertainties in the analysis. Due to these issues, lake liming has not been a widespread practice in North America.

To make liming more accurate, an effective approach is to use time dependent liming where liming decisions (amount of lime to be added) change with time based on the current lake conditions. The reliability of liming can be further improved if these dynamic liming decisions are based on a systematic approach rather than heuristics.

6.1.1. Basic liming model

The basic lake liming model is presented in Ottosson and Hakanson (1997) and further discussed in Hakanson and Boulion (2002) and Hakanson (2003). It is a mixed model consisting of both statistical regression and dynamic interactions. An empirical model is used to predict the initial pH (mean annual pH). The model also includes a regression that predicts natural pH. In addition to these empirical sub-models, the lake liming model consists of dynamic (time dependent) interactions. It is a compartmental model with three different compartments, namely, water, active sediment and passive sediment. Accordingly, the three model variables are: lime in water, lime in active sediment and lime in passive sediment.
Four continuous flows of lime connect the three compartments: sedimentation to active sediments, internal loading from active sediments to water, outflow from the lake water and transport from active to passive sediments. In addition, two flows give the inflow of lime from the liming, one to the lake water and one directly to the active sediments.

Natural pH of a lake varies seasonally and hence constitutes an uncertain parameter. In this work, mean reverting Ito process is used to model fractional variation in pH owing to its success in modeling various time dependent stochastic parameters (Diwekar, 2008; Shastri & Diwekar, 2006a,b).

Optimal control problems require establishing an index of performance for the system and designing the course of action so as to optimize the performance index. The goal in lake liming operation is to maintain the pH value at some desired level or within a desired range. Since cost of liming is also a concern, this converts the problem into multi-objective optimal control problem, where minimization of pH variation and minimization of liming cost are the two objectives.

6.1.2. Results and discussions

Fig. 6 presents the result of deterministic and stochastic optimal control problems indicating that the targeted pH is effectively achieved. The plots also show that the stochastic optimal control leads to better pH control. The steady drift observed while using deterministic control is not a generic result but rather depends on the specific case study and the particular realization of the uncertain variable. The nature of these fluctuations, therefore, may be different for different case studies. However, solutions of different problems showed that the deterministic control is always inferior to stochastic control. The results of the multi-objective optimal control problem, not reported here, show the trade-off between cost and liming accuracy. Such results are very useful to decision-makers to finalize the liming policy as a function of the available resources.

6.2. Manipulation of regime

It has been illustrated that a major portion of mercury found in the tissues of various aquatic organisms enters through food (ingestion). As a consequence, the eating habits of these organisms are expected to have a significant impact on the mercury intake by these organisms. The eating habits depend to quite an extent on the various species populations and their pattern of fluctuations at a given time in the water body. In ecological literature, these different patterns are referred to as regimes. A regime, therefore, if maintained for sufficient duration, is expected to affect the steady state mercury bioaccumulation levels in different species. As a result, manipulation of the regimes of these species populations presents a tool to control mercury bioaccumulation levels (Monson & Brezonik, 1998; Wang, Stupakoff, Gagnon, & Fisher, 1998). This work performs an optimal control analysis to achieve regime shifts for mercury bioaccumulation reduction. The population dynamics in the water body are modeled by a three species predator-prey model (Canale’s model), where the three species are called as prey, predator and super-predator. The bioaccumulation level in the super-predator is of concern for humans since humans often eat those species. Mercury bioaccumulation is modeled using the bioenergetics approach. The predator-prey model and the bioaccumulation model are inter-related by correlating the food intake of any particular species with the mercury intake for the bioaccumulation model. Thus, changes in the dynamics of the Canale’s model change the instantaneous food intake for the predators and super-predators (due to changing predation rates). This affects the total mercury that is taken by these species through food. Hence, any regime shift in the predator-prey model, which affects the predation rates, affects the mercury intake by the species. If the particular regime is maintained for a sufficient duration, the steady state mercury concentration in these species can be altered. This is the basic foundation for the proposed work. It must also be ensured that the new regime is stable and does not compromise the other functions of the system such as primary productivity. Hence, it is very critical to select the right approach to achieve the regime shift. It is also important to note that the total Hg or MeHg levels in the water are not altered. Rather, the objective is to alter the dynamics to ensure lower bioaccumulation levels in the super-predator.

6.2.1. Regime change and optimal control

Optimal control theory presents an option to derive time dependent management strategies that can effectively achieve regime shifts in food chain models. Past work by the authors has illustrated the success of this approach (Shastri & Diwekar, 2006a,b). That work used Fisher information-based sustainability hypothesis, proposed by Fath and Cabezas (2002), to formulate time dependent objective functions for the control problem. That work proved that Fisher information and its variation can successfully be correlated to a specific regime. A similar approach, therefore, has been used in this work. Once the targeted regime with lower mercury bioaccumulation is known, the regime shift is to be achieved by minimizing the variation of the time averaged Fisher information of the system around the constant Fisher information of the targeted regime. Canale’s model exhibits various regimes such as cyclic low frequency, cyclic high frequency, stationary, and chaotic (Gragnani, De Feo, & Rinaldi, 1998; Boer, Kooi, and Kooijman 1998). The idea proposed in this work is to move from a high mercury bioaccumulation regime to a low mercury bioaccumulation regime, both in terms of the super-predator. The control variables to achieve the regime shift are: nutrient inflow rate and nutrient input concentration.

6.2.2. Results and discussion

Fig. 7 shows the regime shift achieved by control of nutrient input concentration for the integrated model (Canale’s model and the bioaccumulation model). The results illustrate that there is a strong correlation between the regime and steady state mercury bioaccumulation in predator and super-predators. Hence, the objective of causing a regime change in justified. In addition to this, the Fisher information-based objective and optimal control theory is successful in driving the system to the desired regime. Moreover, since the new regime is stable, the bioaccumulation level is expected to stay at the new level until the whole system is perturbed beyond the resilience limits. The control profile has not been reported in the interest of space. However, it is observed that the nutrient inflow concentration increases on an average basis for the
simulation horizon. Once the new regime is achieved, the control variable can be maintained at a constant value to ensure that the system remains in the same regime.

7. Summary and conclusion

The primary objective of this work is to emphasize the role of an integrated systems theory-based approach to address issues in green process design, green energy leading towards overall sustainability. This includes not only the traditional process engineering related issues such as product and process design, but also the associated ecological and social aspects. This requires integration and application of various systems theory-based approaches, and some of the important ones are presented in this paper. It is mentioned that the role of uncertainty is important in this analysis to ensure robust results. The paper then analyzes the case of mercury pollution management and illustrates how these concepts can be applied to a real and existing problem. The role of pollutant trading at the industrial sector level is discussed to achieve compliance at reduced financial and social costs. Moreover, the role of liming and systematic manipulation of aquatic population at the ecosystem level is analyzed to further mitigate the harmful impacts of mercury pollution. It is proposed that both of these approaches should be synergistically explored for the mercury pollution management problem. Thus, application of liming for a watershed will have an impact on the final regulation such as TMDL, which in turn will affect the trading decisions. Ultimately, a multi-objective optimization problem as considered in level 5 of the proposed approach, will be formulated that will juxtapose the economic objectives with social and environmental performance indicators. Only an integrated analysis, such as the one proposed here, will be able to look at these inter-dependencies and hence determine the globally optimal solution. Although the specific management options discussed here pertain to mercury pollution, it is proposed that similar approaches should be explored for other issues in the field of sustainability. That is where the role of systems theory and analysis as a tool becomes very valuable.

References


