**OPTIMIZATION METHODS FOR SUSTAINABILITY**

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**Introduction**

Achieving sustainable development by balancing the long-term economic, environmental, and social objectives is one of the most complex scientific problems of our times. From an engineering perspective, translating the concepts of sustainability into decision making is particularly critical. This decision making could be in the form of a design decision or management/policy recommendation. This challenge goes beyond the traditional areas of process development, process design, and industrial ecology, and encompasses multi-scale phenomena and complex interactions of multiple disciplines.

Systems theory is a valuable tool since it enables the integration of these multi-scale, multi-disciplinary components using an informational and computational platform. The various systems theory based tools include modeling, simulation, optimization, and control, which can be used to solve problems in process design, process synthesis, advanced control, fault detection and diagnosis, state estimation and more.

The focus of this module is to illustrate the application of optimization and optimal control theory to solve problems in sustainable design. The module considers the problem of managing mercury waste as a case study and illustrates the application of optimization and optimal control tools at various scales of the problem. It must be noted that most of the systems have some uncertainties associated with them. The uncertainty could be due to the inherent stochasticity of the system, such as weather or rainfall events, or due to our lack of accurate information due to measurement limitations, such as rate constants of a reaction. The uncertainty could also manifest itself when models and data are translated across multiple scales, for example experimental data from lab scale to commercial scale. Therefore, it is important have tools that can systematically incorporate uncertainties in decision making. Therefore, as part of this module, we also discuss the application of stochastic optimization and stochastic optimal control to solve problems in sustainable design of stochastic systems.

**Rationale: Optimization Methods for ensuring Sustainable Engineering**

Optimization has played a crucial role in engineering design over several decades. Optimization theory has been used extensively in areas such as process design, process synthesis, supply chain design and management, and so on within the domain of chemical engineering and manufacturing sector. The challenge of incorporating sustainability in engineering adds more complexity to the decision making process. Optimization theory and methods provide a systematic way of exploring the decision making space and determining the best solution for a particular objective. Therefore, optimization methods are even more important for sustainable engineering. The theory of optimization has been extended to dynamic systems in the form of optimal control theory. Since the consideration of natural systems, which are inherently dynamic in nature, is important for sustainability, the role of optimal control theory becomes evident.

Most of the problems dealing with sustainability involve several uncertainties, and the role of uncertainty increases with increasing spatial and temporal (Figure 1). Therefore, it is necessary to incorporate these uncertainties in decision making. The theory of stochastic optimization and stochastic optimal control, extensions of their deterministic counterparts, provides such as framework. Therefore, knowledge of these methods is also important for sustainable engineering decision making.

Sustainability.tif  
Figure 1: Multi-scale problem of sustainable engineering. The impact of uncertainty increases with increasing spatial and temporal scale

**Methodology and Theory**

**Numerical optimization**

A general optimization problem can be stated as follows.

The goal of an optimization problem is to determine the decision variables x that optimize the objective function Z, while ensuring that the model operates within established limits enforced by the equality constraints ***h*** and inequality constraints ***g***.

Figure 2 illustrates schematically the iterative procedure employed in a numerical optimization technique. As seen in the figure, the optimizer invokes the model with a set of values of decision variables x. The model simulates the phenomena and calculates the objective function and constraints. This information is utilized by the optimizer to calculate a new set of decision variables. This iterative sequence is continued until the optimization criteria pertaining to the optimization algorithm are satisfied.

There are a large number of software codes available for numerical optimization. Examples of these include solvers such as MINOS, CPLEX, CONOPT, and NPSOL. Also, many mathematical libraries, such as NAG, OSL, IMSL, and HARWELL have different optimization codes embedded in them. Popular software packages such as EXCEL, MATLAB, and SAS also have some optimization capabilities. There are algebraic modeling languages like AMPL, LINGO, AIMMS, GAMS, and ISIGHT specifically de- signed for solving optimization problems and software products such as Omega and Evolver have spreadsheet interfaces. However, a discussion of all the different accessible software is beyond the scope of this book. SIAM publications provide a comprehensive software guide by More and Wright (1993).

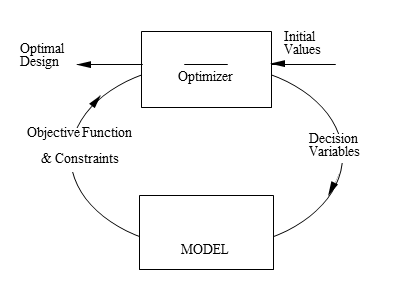


Figure 2: Pictorial representation of the numerical optimization framework

Furthermore, the Internet provides a great source of information. A group of researchers at Argonne National Laboratory and Northwestern University launched a project known as the Network-Enabled Optimization System (NEOS). Its associated Optimization Technology Center maintains a Web site at: <http://www.mcs.anl.gov/otc/> which includes a library of freely available optimization software, a guide to software selection, educational material, and a server that allows online execution. Also, the site: <http://OpsResearch.com/OR-Objects> includes data structures and algorithms for developing optimization applications.

Optimization algorithms mainly depend upon the type of optimization problems described in the next section.

**Types of optimization problems**

Optimization problems can be divided into the following broad categories depending on the type of decision variables, objective function(s), and constraints.

* Linear programming (LP): The objective function and constraints are linear. The decision variables involved are scalar and continuous.
* Nonlinear programming (NLP): The objective function and/or constraints are nonlinear. The decision variables are scalar and continuous.
* Integer programming (IP): The decision variables are scalars and integers.
* Mixed integer linear programming (MILP): The objective function and constraints are linear. The decision variables are scalar; some of them are integers while others are continuous variables.
* Mixed integer nonlinear programming (MINLP): A nonlinear programming problem involving integer as well as continuous decision variables.
* Discrete optimization: Problems involving discrete (integer) decision variables. This includes IP, MILP, and MINLPs.
* Optimal control: The decision variables are vectors.
* Stochastic programming or Stochastic Optimization: Also termed optimization under uncertainty. In these problems, the objective function and/or the constraints have uncertain (random) variables. Often involves the above categories as subcategories.
* Multiobjective optimization: Problems involving more than one objective. Often involves the above categories as subcategories.

Type of optimization problem decides the method for solution as optimality conditions change for different optimization problems.

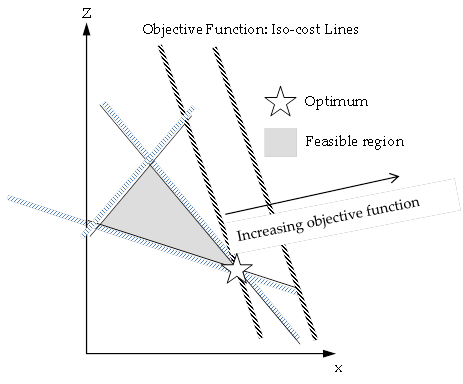


Figure 3: A Linear Programming Problem

Figure 3 plots the graph of the objective function Z versus a decision variable x. Figure 3 shows a linear programming problem where the linear objective function as well as its constraints (lines AB, BC, and CA) are linear. The constraints shown in Figure 1.2 are inequality constraints indicating that the solution should be above or on line AB, and below or on lines BC and CA. ABC represents the feasible region of operation within which the solution should lie. The constraints are binding the objective space, and hence the linear objective is lying at the edge of the feasible region (constraint). LP optimum lies at the vertex of the feasible region and is the basis of simplex method for solving LP problems.

Figure 4 shows an unconstrained (a) and a constrained (b) nonlinear programming problem. In the unconstrained problem the feasible region extends to infinity. The minimum of the objective function lies at point B, where the tangent to the curve is parallel to the x-axis, having a zero slope (the derivative of the objective function with respect to the decision variable is zero). The optimality conditions for an NLP are based on gradients of objective function and constraints. For the constrained NLP shown in Figure 4 b, the optimality condition is found by balancing the gradients of the objective function and constrained. Where the linear equation of gradients (KKT conditions) is zero, the optimum lies.

It can be seen the optimality conditions for different types of problems are different. For discrete optimization which involves integer variables. Optimal solution can be found using heuristic and bounding information, coupled with LP, NLP techniques depending upon the type of problem (IP, MILP, or MINLP).

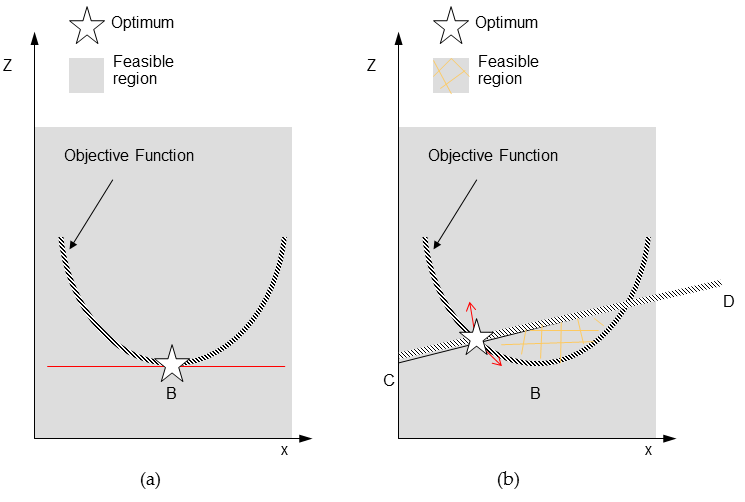


Figure 4: A nonlinear programming problem

Optimal control problems are the most difficult problems in deterministic optimization. They involve differential algebraic equations and vector decision variables. There are number of solution methods available to solve these problems but involves transformation of the problem. These are given below.

* Calculus of variations or variational calculus
  + Transforms the problem into second order differential equations.
* Pontryagin’s maximum principle
  + Involves adding adjoint variables and adjoint ordinary differential equations
  + Involves two point boundary value problem
* Dynamic programming
  + Transforms the problem into equivalent partial differential equations based on principle of optimality.
* NonLinear Programming
  + Involves discretization of differential equations
  + Results in a large NLP optimization problem

So far, we have discussed deterministic optimization techniques. In stochastic optimization or stochastic programming, the objective function and constraints are probabilistic. These problems involve adding a stochastic modeling loop for various samples or scenarios for uncertainty analysis as shown in Figure 5. The methods for stochastic optimization/programming are derived from their deterministic equivalents.

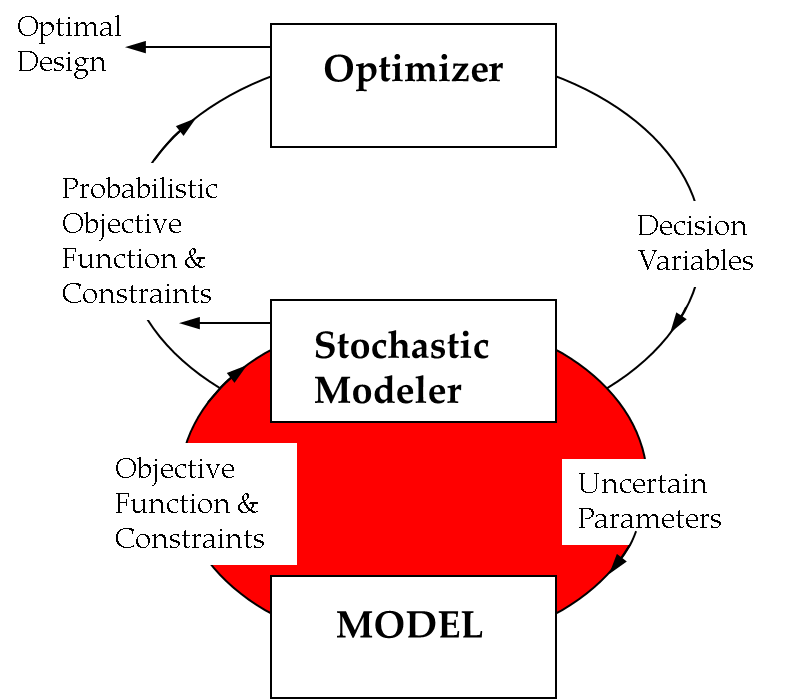


Figure 5: Schematic of Stochastic Optimization or Stochastic Programming Problem

Multi-objective optimization involves two kinds of methods, namely, the preference based methods, or the generating methods. In preference based methods, a single objective problem is derived from stake holders’ preferences. This problem can then be solved using traditional LP, NLP, or Mixed integer methods as prescribed by the problem. Generating methods involve solution of number of single objective problems derived to find the Pareto surface. Again the optimality criteria for these single objective problems are based on whether the problem is LP, NLP, or mixed integer problem.

**Optimization approach to sustainability**

Optimization has been a valuable tool in designing and operating plants. In sustainable manufacturing, environmental and societal considerations are included not merely as constraints, but are part of the objective function. Thus, it is a multi-objective optimization problem. In order to include decisions starting from discovery stage and include various objectives at the other end, an optimization framework which includes discrete decision making for decisions like selection of material, selection of equipment and continuous decisions like material flow needs to be considered. A framework presented by Diwekar and co-workers (Diwekar, 2003) are shown in Figure 6 and is described below.

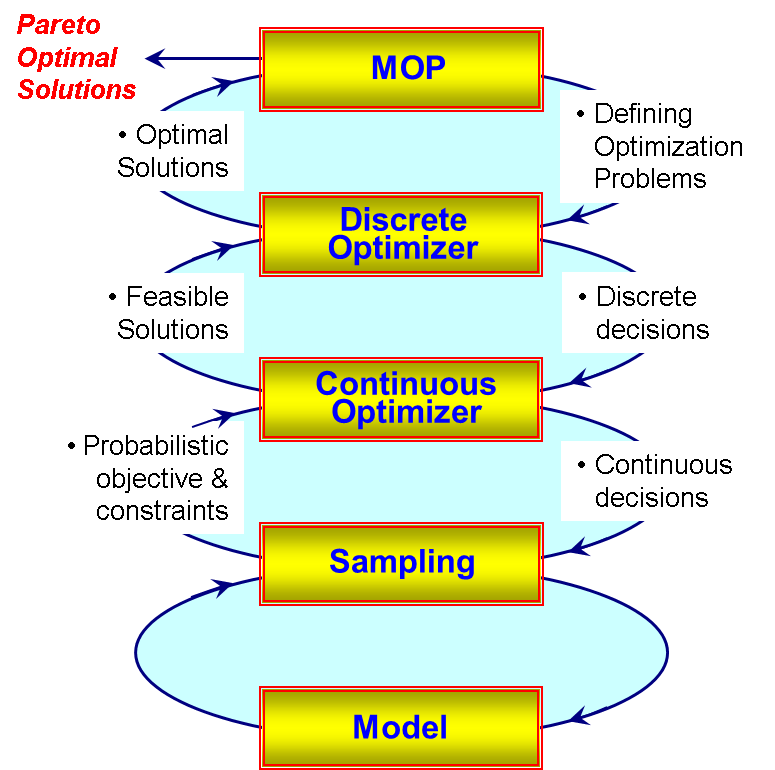


Figure 6: Optimization Framework for Sustainable Manufacturing (Diwekar, 2003)

**Level 1**, is the inner most level and corresponds various models like material and energy balances, equipment design equations, and models for impact assessments. Obviously these models come from various disciplines like engineering, ecology, economics, social sciences, and policy analysis. The multi-disciplinary multi-scale nature of the modeling poses number of challenges.

**Level 2, Sampling loop**. The diverse nature of uncertainty, such as estimation errors and process variations, can be specified in terms of probability distributions. 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. Sampling is a major bottleneck in the computational efficiency of the stochastic programming (optimization under uncertainy) problems. One of the most widely used techniques for sampling from a probability distribution is the Monte Carlo sampling technique. Latin hypercube sampling (McKay et al., 1979; Iman and Conover, 1982) is one form of stratified sampling that can yield more precise estimates of the distribution functions than Monte Carlo. However, the main drawback of this stratification scheme is that it is uniform in one dimension and does not provide uniformity properties in k-dimensions. Efficient sampling techniques (Hammersley sequence sampling and Latin Hypercube Hammersley Sampling) based on Hammersley points have been proposed by the Diwekar and co-workers (Kalagnanam and Diwekar, 1997; Wang et al., 2004) use optimal design schemes for placing the n points on a k-dimensional hypercube. These schemes ensure that the sample set is more representative of the population, showing uniformity properties in multi-dimensions, unlike Monte Carlo, Latin hypercube, and its variant, the Median Latin hypercube sampling technique. It has been found that the HSS and LHHS techniques are an order of magnitude faster than LHS and Monte Carlo techniques and hence, they are the preferred techniques for uncertainty analysis, as well as optimization under uncertainty.

**Level 3, Continuous optimizer.** This step involves decisions regarding design and operating conditions of the plant. These are continuous decisions and requires techniques for LP, NLP, SLP, SNLP from the optimization literature. For details please refer to Diwekar (2008).

**Level 4, Discrete optimizer.** Discrete decisions like selection of material, selection of equipments and their order are decided at this level. There are number of approaches for discrete optimization. Traditional Mixed Integer NonLinear Programming (MINLP) methods use open equation system. For global optimization and black box models probabilistic methods like simulated annealing, genetic algorithm, ant colony optimization can be used. For details of these methods, please refer to Diwekar (2008).

**Level 5: Multi-objective Optimization**. It 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. For each of these decisions, it is impossible to improve one objective without sacrificing the value of another relative to some other alternative in the set. It is then the decision maker who decides which solutions of the Pareto set to considered. There are two types of generating methods available for this, namely, the weighting method and the constraint method. In weighting method, a single objective is formed by weighting various objective function, and optimization problem is solved using sets of different weights to obtain Pareto surface. In constraint method, the basic strategy is also to transform the multi-objective optimization problem into a series of single objective optimization problems. The idea is to pick one of the objectives to minimize (say Zl) while each of the others (Zi, i = 1, . . ., k, i ≠ l) is turned into an inequality constraint with parametric right-hand sides (εi, i = 1, . . ., k, i ≠ l). Solving repeatedly for different values of εi, . . ., εl−1, \_l+1, . . ., εk leads to the Pareto set. Alternative to generating method is goal programming method, which sets goals for different objective, and a single solution is then obtained. The challenge in sustainability is to define the proper objectives for this framework.

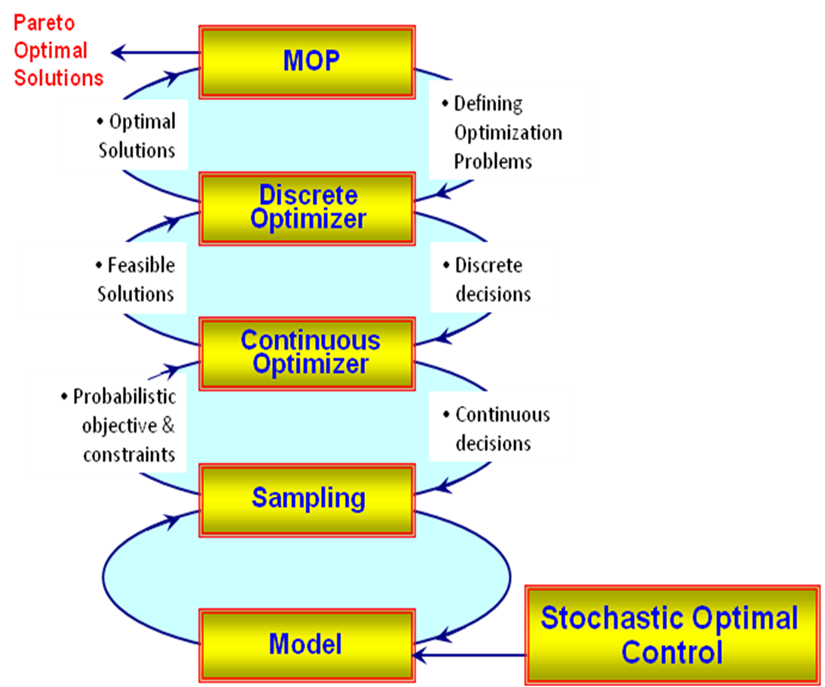


Figure 7: Optimization Framework for Sustainability (Diwekar and Shastri, 2010)

Although this framework is useful for obtaining greener designs and operating conditions at the plant level, as stated earlier for industrial ecology and ecosystem sustainability, we need to consider time dependent uncertainties and time dependent decisions. Diwekar and co-workers modified the framework shown in Figure 6. Figure 7 shows this new framework (Diwekar and Shastri, 2010). In this framework, time dependent decisions and time dependent uncertainties are handled by optimal control and stochastic optimal control methods (Diwekar, 2008).

**Case Study: Mercury Waste Management**

This module illustrates the application of optimization and optimal control theory for sustainability. To achieve this goal, we will discuss the theme of mercury waste management. Mercury waste, in addition to being an important environmental problem created by anthropogenic actions, also manifests itself over several spatial and temporal scales. Therefore, it aligns well with the multi-scale nature of sustainability emphasized in Figure 1.

Mercury has been recognized as a global threat to our ecosystem, and it is fast becoming a major concern to environmentalist and policy makers. Mercury is a major pollutant from coal based power plants. The task of mercury pollution management is arduous due to the complex environmental cycling of mercury compounds. Mercury can cycle in the environment in all media as part of both natural and anthropogenic activities.

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. These point sources of mercury need to be regulated to reduce the final emission into the atmosphere. This can be achieved by plant level interventions such as better process design and operations or use of more efficient control technologies such as mercury capture in power plants. This would fall under the domain of green design.

The point sources of mercury are often required to limit the total emissions to a particular level as per the regulatory guidelines. However, different point sources often incur different marginal cost for the reduction of same amount of mercury pollutant. Pollutant trading is a market based approach which aims to achieve the same or better environmental performance with respect to pollution management at a lower overall cost. The relative success of this approach for air pollutants [4, 5, 6, 7], including the USEPA issued federal rule in 2005 allowing cap and trade policy to reduce mercury emissions from coal-fired power plants, has encouraged the introduction of watershed based pollutant trading [8, 9]. It is expected that pollutant trading will reduce the overall compliance costs for an industrial sector. Therefore, it represents the industrial symbiosis or industrial ecology dimension of sustainability (Figure 1).

The impact of pollutant trading on the overall mercury emissions needs to be considered. Here, the impact on human health through exposure to mercury is important. Since the emissions cannot be completely stopped, the allowable emission limit indirectly puts a value to the human life. This, therefore, becomes a regulatory and policy issue (Figure 1). The trading mechanism needs to consider these factors in decision making.

Most of the mercury emitted 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 waste water 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. The consumption of these aquatic animals by humans and wild animals further aids 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. We, thus, need to explore options to limit the impact of mercury already present in the ecosystem. Therefore, ecological level interventions, such as lake liming, are proposed.

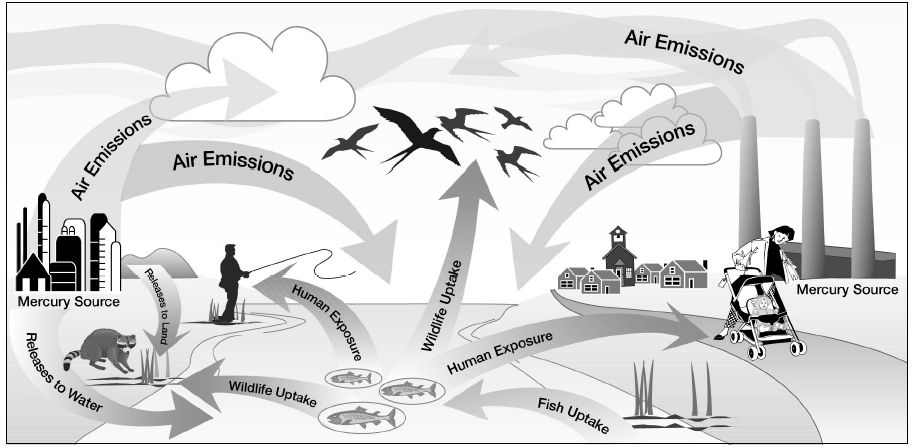


Figure 8: Biogeochemical cycling of mercury in the atmosphere (Adapted from Mercury Research Strategy USEPA)

The complete module is divided into five cases. In Case Study 1, the application of optimization to a pulverized coal power plant developed in ASPEN Plus simulation software is presented. In Case Study 2, the selection of the optimal mercury control treatment technology for industries discharging mercury waste in water is discussed. In Case Study 3, the application of mercury trading at the industrial sector level for mercury management, with considerations of health care costs and uncertainties, is discussed. In Case Study 4, the application of optimal control theory for control of lake pH using lake liming is discussed. Finally, in Case Study 5, the deterministic optimal control problem is extended to consider uncertainties in natural pH variations, thereby formulating a stochastic optimal control problem.

**Connections to Existing Core Curriculum**

Most of the existing chemical engineering undergraduate core curriculums involve a basic course on process control. Moreover, most departments also offer courses on optimization, modeling and simulation, as well as waste management. Sustainability is also increasingly being brought into focus in the existing courses. In that regard, this module provides a useful source for students to understand how the knowledge gained through other courses can be used to solve multi-scale problems in sustainability.

**References and Further Reading**

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