Computers and Chemical Engineering 34 (2010) 1348–1355

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

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

Urmila M. Diwekar*, Yogendra N. Shastri

Center for Uncertain Systems: Tools for Optimization & Management, Vishwamitra Research Institute, Clarendon Hills, IL 60514, United States

ARTICLE INFO

Article history:
Received 4 August 2009
Received in revised form
29 December 2009
Accepted 12 February 2010
Available online 20 February 2010

Keywords:
Green process design
Green energy
Sustainability

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 and 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.

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 non-equilibrium-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-

* Corresponding author at: CUSTOM, Vishwamitra Research Institute, 368 56th Street, Clarendon Hills, IL 60514, United States. Tel.: +1 630886 3047.
E-mail address: urmila@vri-custom.org (U.M. Diwekar).

0098-1354/$ – see front matter © 2010 Elsevier Ltd. All rights reserved.
doi:10.1016/j.compchemeng.2010.02.010

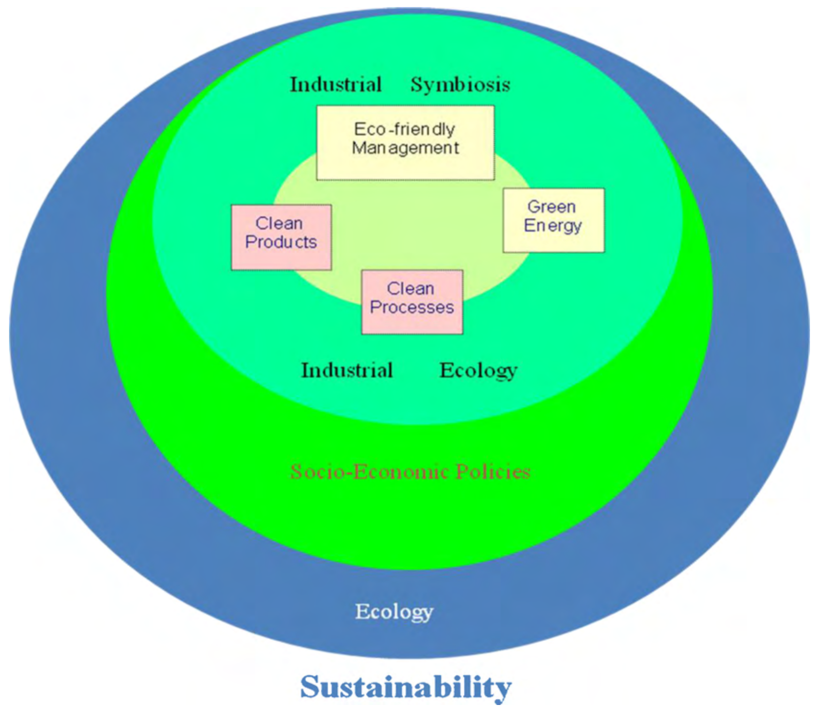

Fig. 1. Green design to industrial ecology to sustainability.

sion is necessary to justify the proposed integrated algorithmic framework that is subsequently described in the article.

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